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DEPARTMENT OF ELECTRICAL AND ELECTRONIC ENGINEERING

**Bipolar Resistive Switching of Bi-Layered Pt/Ta₂O₅/TaO_x/Pt
RRAM – Physics-based Modelling, Circuit Design and Testing.**

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LIST OF ABBREVIATIONS

Acronym	Description
NVM	Non-Volatile Memory
MRAM	Magnetic Random Access Memory
PRAM	Phase-Change Random Access Memory
FRAM	Ferroelectric Random Access Memory
SRAM	Static Random Access Memory
DRAM	Dynamic Random Access Memory
RRAM	Resistive Random Access Memory
RS	Resistive Switching
BRS	Bipolar Resistive Switching
NV	Non-Volatile
MIM	Metal-Insulator-Metal
MISM	Metal-Insulator-Semiconductor-Metal
HRS	High Resistance State
LRS	Low Resistance State
TEM	Transmission Electron Microscopy
TPF	Tunnelling Probability Factor
CF	Conductive Filament
HSV	High Resistance State Switching Voltage
BE	Bottom Electrode
TE	Top Electrode
AFM	Atomic Force Micrograph
LSV	Low Resistance State Switching Voltage
VCCS	Voltage-Controlled Current Source
VCVS	Voltage-Controlled Voltage Source
OCF	Outside the CF

LIST OF PUBLICATIONS

Peer Reviewed Journal Articles

1. **F. O. Hatem**, T. N. Kumar, and H. A. F. Almurib, “A SPICE Model of the Ta₂O₅/TaO_x Bi-Layered RRAM,” *IEEE Transactions on Circuits and Systems I: Regular Papers*, vol. 63, no. 9, pp. 1487–1498, Sept. 2016.
2. **F. O. Hatem**, P. W. C. Ho, T. N. Kumar, and H. A. F. Almurib, “Modeling of bipolar resistive switching of a nonlinear MISM memristor,” *Semiconductor Science and Technology*, vol. 30, no. 11, p. 115009, Oct. 2015.
3. P. W. C. Ho, **F. O. Hatem**, T. N. Kumar, and H. A. F. Almurib, “Comparison between Pt/TiO₂/Pt and Pt/TaO_x/TaO_y/Pt based Bipolar Resistive Switching Devices,” *J. Semicond.*, vol. 37, no. 6, p. 064001, June 2016.

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4. P. W. C. Ho, **F. O. Hatem**, T. N. Kumar, and H. A. F. Almurib, “Enhanced SPICE memristor model with dynamic ground,” in *Proc. IEEE Int. Circuits and Syst. Symposium*, Sep. 2015, pp. 130-132.
5. P. W. C. Ho, **F. O. Hatem**, T. N. Kumar, and H. A. F. Almurib, “Comparison on TiO₂ and TaO₂ based bipolar resistive switching devices,” in *Proc. 2014 2nd Int. Conference on Electronic Design*, Aug. 2014, pp. 249-254.

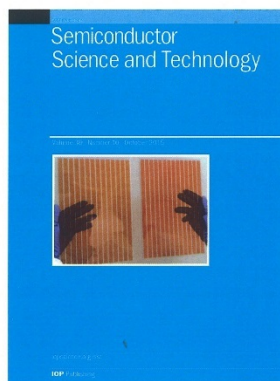
Peer Reviewed Poster Presentations

6. **F. O. Hatem**, T. N. Kumar, and H. A. F. Almurib, “Ph.D Thesis: Bipolar Resistive Switching of Bi-Layered Pt/Ta₂O₅/TaO_x/Pt RRAM–Physics-based Modelling, Circuit Design and Testing,” in *Design, Automation & Test in Europe Conference and Exhibition (DATE)*, Lausanne, Switzerland, Mar. 2017.

Publications in Preparation

7. A journal paper titled “Compact SPICE Model of Ta/TaO_x/Pt MIM RRAM” is currently in preparation and will be submitted to one of the related journals.
8. A conference paper based on using the proposed bi-layered RRAM SPICE model developed during this research in a RRAM-based circuit application. The paper will be submitted for presentation to an IEEE related conference.

LIST OF AWARDS



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ABSTRACT

Over the last few years, the non-volatile memories (NVM) have been dominating the research of the storage elements. The resistance random-access memory (RRAM) and the memristor that employs the resistive switching (RS) mechanism appear to be potential candidates for NVM. Among the RS materials that were reported is the TaO_x which showed surprising RS performance. This oxide material has been widely used to construct a metal-insulator-semiconductor-metal (MISM) RRAM which can be referred to as bi-layered RRAM. This bi-layered RRAM consists of TaO_x as a bulk material and Ta_2O_5 as an insulator layer, sandwiched between two platinum electrodes to form $\text{Pt}/\text{Ta}_2\text{O}_5/\text{TaO}_x/\text{Pt}$ RRAM. However, a physics-based mathematical model of this RRAM is required to further study the detailed physics behind its conduction mechanism and the RS process. In addition to the mathematical model, a SPICE model is also required to understand the behaviour of this bi-layered RRAM device when integrated in memory design for the future generation storage devices or when used in RRAM-based circuit applications.

This doctoral research presents novel mathematical and SPICE models of a bipolar resistive switching (BRS) of the $\text{Pt}/\text{Ta}_2\text{O}_5/\text{TaO}_x/\text{Pt}$ bi-layered RRAM. For this purpose, MATLAB and LTSPICE are used to design the mathematical and the SPICE bi-layered RRAM models, respectively, and the obtained simulation results for both models are compared with the experimental data from SAMSUNG labs.

The novelty of the mathematical model lies in incorporating the tunnelling probability factor (TPF) between the semiconductor and the metal layers and therefore, demonstrating its effect on the conduction mechanism. In addition, the effect of continuous variation of the interface traps densities and the ideality factor during BRS is modelled using the semiconductor properties and

the characteristics of the metal-insulator-semiconductor (MIS) system. Thus, the model emphasizes the dependency of the device current on the physical characteristics of the insulator layer. Moreover, the electric field equation for the active region is derived for the MISM structure which is used together with Mott and Gurney rigid point-ion model and Joule heating effect to model the oxygen ion migration mechanism. Finally, the model also demonstrates the self-limiting growth of the doped region.

The proposed SPICE model emphasizes the impact of the change in the switching layer thickness on the device behaviour at low resistance state (LRS), high resistance state (HRS), and the transitional period. The validity of the SPICE model is verified through using three different sets of experimental data from Pt/Ta₂O₅/TaO_x/Pt RRAM with switching layer thickness smaller than 5 nm. The SPICE model reproduced all the major features from the experimental results for the SET and RESET processes and also the asymmetric and the symmetric characteristics in HRS and LRS, respectively. The SPICE model matches the measured experimental results with an average error of < 11%. It also showed stable behaviour for its HRS and LRS regions under different types of input signals. The model is parameterized in order to fit into Ta₂O₅/TaO_x RRAM devices with switching layer thickness smaller than 5 nm, thus, facilitating the model usage. The SPICE model can be included in the SPICE-compatible circuit simulation and is suitable for the exploration of the Ta₂O₅/TaO_x bi-layered RRAM device performance at circuit level.

At the end of the research, a metal-insulator-metal (MIM) RRAM SPICE model of Ta/TaO_x/Pt is developed which can be used in the future work to compare between the MISM and MIM TaO_x-based RRAM devices.

INTRODUCTION

1.1. Resistive Random Access Memory Devices

Over the last few years, the non-volatile memories (NVM) have been dominating the research of the storage elements [1], [2]. Examples of such memories are the magnetoresistive random-access memory (MRAM) [3], phase-change random-access memory (PRAM) [4], and ferroelectric random-access memory (FRAM) [5]. These candidates aim for the replacement of the conventional semiconductor memories such as Si charge-based flash memory, static random-access memory (SRAM), and dynamic random-access memory (DRAM) [6]. However, considering the future NVM at nanoscale range requires switching mechanism to be operating in the range of at least 10–30 nm technology with switching current in the range of 10–100 μA [1], PRAM has a problem with the switching current condition [4] while FRAM and MRAM appear to have limitations with the scaling [5]. At the same time, the flash memory has also been lacking in achieving some of the important future NVM requirements (e.g., switching speed, retention time, and the number of WRITE–ERASE cycles) [1].

Alternatively, metal-oxide bipolar resistive random-access memory (RRAM) and the memristor that employs resistive switching (RS) mechanism appear to be a potential candidates for the next generation NVM [1], [7], [8], [9] and their applications [10], [11], [12], [13]. RRAM devices can be considered as a specific type of the memristors which can describe the bipolar resistive switching (BRS) behaviour [9], [14]. RRAM devices demonstrate various characteristics and attributes which make it useful element for logic circuit design, neuromorphic systems, and memory applications such as high density cross bar memories. For example, RRAM provide non-volatile (NV) characteristics, fast write and read time and it has a non-destructive reading mechanism where the stored data is ideally not altered (or slightly altered) during the reading mechanism [15]. RRAM devices exhibit the non-destructive behaviour because its state variable change slightly in the case of low current (reading current) while the change due to high current is significantly larger. In other words, the RRAM state variable has a nonlinear dependence on the charge [15]. In addition, RRAM provides high $R_{\text{OFF}}/R_{\text{ON}}$ ratio in order to store distinct Boolean data where R_{OFF} and R_{ON} are the RRAM resistances at high resistance state (HRS) and low resistance state (LRS), respectively. In general, when storing a digital state into a certain memory device, it is important for the stored data to be distinct. This means that the differences between the stored data are considerably large. By doing this, we guarantee that the digital stored state is not sensitive to the changes in both the operating conditions and the parameters [15]. In addition to these characteristics, RRAM devices demonstrate a good scalability and low power consumption.

Knowing that the RRAM devices exhibit all these useful characteristics which makes it an important device for the potential circuits applications, especially NVM, a great appreciation

and interest has been developed in this field which led to the start of this doctoral research. Also, knowing that the leading companies in the field (SAMSUNG, Hewlett Packard, Micron, IBM, Panasonic...etc.) are currently carrying out research and developments on these promising memory candidates, an excellent research opportunity arises for conducting more explorations and experiments in this promising field.

1.2. Research Gap in the Field of RRAM Devices

Based on their structure, RRAM devices can be classified into metal-insulator-metal (MIM) [7] and metal-insulator-semiconductor-metal (MISM) RRAM devices [1], [8] hereafter will be referred to as bi-layered RRAM. A typical tantalum oxide-based MISM and MIM RRAM physical devices are shown in Figure 1.1(a) and (b), respectively [16].

Recently, the bi-layered RRAM has been extensively studied as one of the promising candidates for the NVM [1], [8], [16], [17], [18], [19], [20], [21], [22], [23], [24], [25], [26]. As can be seen in Figure 1.1(a), typical bi-layered RRAM device comprises a bulk layer and a more RS oxide layer, sandwiched between two metal electrodes [8]. Different RS oxide materials have been reported for the bi-layered RRAM devices such as: AlO_x/WO_x [22], CuO/ZnO [23], $\text{HfO}_x/\text{AlO}_x$ [24] and [25], $\text{TiO}_x/\text{HfO}_x$ [26], and $\text{Ta}_2\text{O}_5/\text{TaO}_x$ [1], [8], [16], [17], [18], [19], [20], [21]. Among these materials, Ta_2O_5 is considered as one of the prospective RS materials which attracted increasing research interest and showed surprising performance. In particular, it exhibited an extreme cycling endurance of over 10^{12} , an improved retention time of more than 10 years, an abrupt switching time (< 1 ns), multilevel states, two stable phases

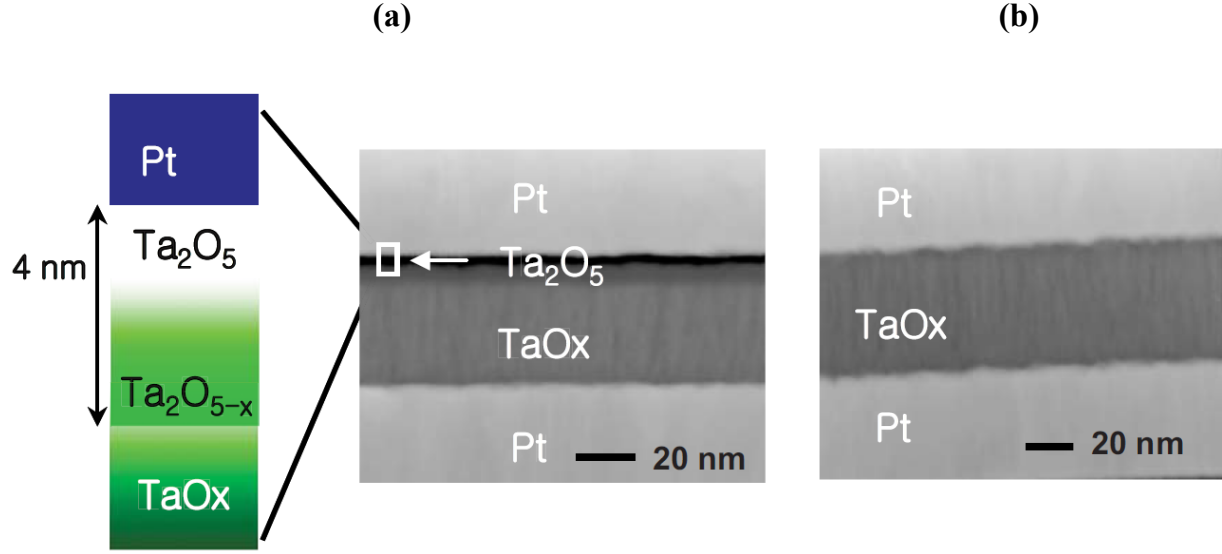


Figure 1.1. Transmission Electron Microscopy (TEM) image of (a) Pt/Ta₂O₅/TaO_x/Pt bi-layered RRAM film and (b) Pt/TaO_x/Pt MIM RRAM film [16].

of TaO_x and Ta₂O₅ [27], [28], and good scalability for the potential applications [1], [29], [30], [31].

Due to these promising RS characteristics of the Ta₂O₅ oxide material, the researchers have adopted the Pt/Ta₂O₅/TaO_x/Pt as one of the potential bi-layered RRAM devices where TaO_x acts as a bulk material and Ta₂O₅ as an insulator layer, forming MISM structure [1], [16], [29] [see Figure 1.1(a)].

However, to facilitate the electrical characteristics of the Ta₂O₅/TaO_x bi-layered RRAM in the simulation environment, a mathematical model that explains the physics involved in its current conduction and RS processes is required. Such model is still missing in the literature and the task of developing this model led to the first stage of the research (Chapter Four). In addition, for the developed Ta₂O₅/TaO_x bi-layered RRAM mathematical model to be useful for the design and performance evaluation of the RRAM-based circuit applications, a reliable and

predictive SPICE model of this device is required which also still missing in the available literatures. The task of developing this RRAM SPICE model led to the second stage of this research (Chapter Five).

1.3. Motivation and Contributions to Develop a Mathematical Bi-Layered Ta₂O₅/TaO_x RRAM Model–Research First Stage

Despite the advances in the Ta₂O₅/TaO_x bi-layered RRAM models [8], [16], [17], [18], [19], [20] and other bi-layered RRAM models based on different materials (e.g. Al/AlO_x/WO_x/W) [22], a new physics-based mathematical model is required to further study the detailed physics behind the conduction mechanism (static behaviour) and the evolution of the doped region (dynamic behaviour) in the Ta₂O₅/TaO_x bi-layered RRAM. In the first stage of this research, a novel physics-based model that describes the BRS behaviour in the Ta₂O₅/TaO_x bi-layered RRAM is presented (Chapter Four). The proposed model is developed based on the MIS system behaviour. It also comprises the physical characteristics of the Ta₂O₅ insulator layer by considering: (1) The tunnelling probability factor (TPF) and (2) The continuous charging and discharging of the interface traps. In addition, the proposed model also (3) derives the electric field equation for the ions hopping switching region in order to predict the oxygen ion migration mechanism. The main three contributions of the first stage are listed below.

1.3.1. Modelling of TPF

At high field, the presence of the insulator layer in the MIS system has certain effects on the device behaviour. First, it leads to the modification the TPF: a term in the current conduction

equation of the MIS system which is used to determine the tunnelling current probability in the device and was reported in [32]. TPF will depart from 1 (indicates ideal Schottky barrier conduction) to smaller value to emphasize the occurrence of tunnelling [32]. It has been theorized in [32] that the tunnelling can occur in an insulator layer of few nanometer thickness only. According to [17], the usual thickness of the insulator layer in the Ta₂O₅/TaO_x RRAM is 2–5 nm which is in the reasonable range for the tunnelling to occur [32]. TPF has not been considered by the previous Ta₂O₅/TaO_x bi-layered RRAM models and also the bi-layered RRAM models based on other materials. As TPF reduces the RRAM current significantly, including it in the current equation becomes vital. Therefore, in the mathematical model developed in the first stage of this research, a different approach than the one presented in the previously reported Ta₂O₅/TaO_x RRAM models is used. It is developed by assuming that the carriers can penetrate and pass through the potential barrier (known as tunnelling conduction process) [32], [33].

1.3.2. Modelling the Continuous Charging and Discharging of the Interface Traps

Besides the effect of TPF term, the mathematical model developed in this research exhibits the physical mechanism of the continuous charging and discharging of the interface traps which was reported in [32]. The current–voltage (I – V) behaviour in this model is based on the continuous variation in the interface traps density and hence, demonstrates the impact of the continuously changing value of the ideality factor η along RS cycles.

1.3.3. Modelling of Electric Field and Ions Migration Mechanism

The third task in the first stage is to derive the average electric field equation for the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM and use it together with Mott-Gurney rigid-point ion model and Joule heating effect to model the actual nonlinear ionic drift behaviour of the oxygen ions. This is achieved by modelling the actual voltage drop on the active region of ions hopping in the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM. Due to the modelling of the electric field and the doped region dynamics, the self-limiting growth of the doped region has also been demonstrated in the bi-layered RRAM mathematical model developed during this research.

To the best of the researcher's knowledge, this is the first physics-based bi-layered RRAM mathematical model (of $\text{Ta}_2\text{O}_5/\text{TaO}_x$ or other material) that considers all these physics phenomena at the same time during its current conduction and doped region evolution mechanisms. The results obtained in the first stage of this research show that the proposed mathematical model depicted a good agreement with the experimental data and predicted most of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM attributes and properties which further support the correctness of our model. At the end of the first stage, all the MATLAB modelling steps and the obtained results were published in [21].

1.4. Motivation and Contributions to Develop a SPICE $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM Model – Research Second Stage

In order for the bi-layered RRAM mathematical model developed in the first stage of the research to be useful for the design and performance evaluation of the RRAM-based circuit

applications, a reliable and predictive SPICE model that can fit into the measured properties of this device is required.

However, for a truly predictive and accurate RRAM SPICE model, the design should be based (whenever possible) on the accurate physics involved in the device operation. The physics-based modelling approach has been applied to different NVM candidates such as MRAM [34], [35], [36] and RRAM [18], [21], [25]. However, due to the complexity of the physical processes involved in the device operation, coming up with a physics-based model that reproduces the widest set of the device behaviour is very difficult and the final model is less computationally efficient compared to other modelling approaches. The main advantage of the physics-based modelling compared to the other modelling approaches is highly predictive models that do not fail for operation outside the measured data window.

In the second stage of this research (Chapter Five), a physics-based SPICE model that can simulate and match the characteristics of the Ta₂O₅/TaO_x bi-layered RRAM with Ta₂O₅ insulator layer thickness (D) smaller than 5 nm has been developed. The proposed SPICE model is based on the Ta₂O₅/TaO_x RRAM mathematical model developed in Chapter Four. The current conduction in the developed SPICE model is based on Schottky barrier modulation and the tunnelling mechanism. This mechanism reflects the effects of changing D on the current conduction process and can only be used when D is thin enough to allow tunnelling [21], [32]. This is attributed to the change of the conduction mechanism in the RRAM devices based on the oxide layer thickness, which makes it very challenging to develop a universal SPICE model that is suitable for a Ta₂O₅ layer of any given thickness. Besides the conduction process, the RS mechanism in the proposed SPICE model also accounts for the variation of D by using the

electric field of the un-doped region of the conductive filament (CF) in its growth rate equation. The un-doped region is the CF region with low/high concentration of oxygen vacancies/ions (the high resistance region of the CF). At the end of the second stage, all the SPICE modelling steps and the obtained results were published in [37].

1.5. Aims and Objectives of the Research

The aims and objectives of this research are divided into two separate stages where each stage has its investigation lines and objectives as shown below.

1.5.1. Aims and Objectives of the First Stage

The investigation lines of the first stage of the research can be summarized in the following objectives:

- 1- Literature review on the recent developments and researches in the field of RRAM analytical and SPICE modelling, especially, $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM models.
- 2- During literature review stage, a comparison between the existing RRAM models (MIM and bi-layered) and the modelling approach proposed in this research is to be conducted in order to show why a solid mathematical model of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM is required.
- 3- The research is then oriented to consider the physics involved in the RS and the current conduction mechanisms of the of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM device and come with the physics-based equations that can represent this RRAM device behaviour.

- 4- Develop a physics-based mathematical model that can simulate and match the characteristics of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM with insulator layer thickness smaller than 5 nm.
- 5- Verify the obtained simulation results with the experimental results published by SAMSUNG labs for $D = 4\text{nm}$.

1.5.2. Aims and Objectives of the Second Stage

The investigation lines of the second stage of this research can be summarized in the following objectives:

- 1- Develop a physics-based BRS SPICE model of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM. The model can emphasize the impact of the change in the switching layer thickness on the device behaviour at LRS, HRS, and the transitional period. This is achieved by integrating the physics involved when Ta_2O_5 layer thickness is changed. i.e. integrating D and/or w into the electric field equation, Schottky barrier height equation, TPF equation, and the ideality factor equation where w refers to the length of the un-doped region of the CF.
- 2- Design the circuit model in such a way to be parameterized in order to fit into $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM with switching layer thickness smaller than 5 nm, thus, facilitating the model usage.

- 3- Verify the obtained simulation results with the experimental results from SAMSUNG labs for three different sets of experimental data: $D = 3$ nm, $D = 4$ nm and also using different pulse amplitude signals.
- 4- The designed SPICE model is then used for RRAM-based circuit application, providing more flexibility in the used device thickness and the bias signal.
- 5- Developing a SPICE model for the Ta/TaO_x/Pt MIM RRAM based on an existing analytical model. This model can then be used in the future together with the bi-layered SPICE model developed in the second stage to compare the performances between the TaO_x-based MIM and MISM RRAM devices.

1.6. Methodology

1.6.1. Mathematical and SPICE Modelling

- 1- A physics-based mathematical Pt/Ta₂O₅/TaO_x/Pt RRAM model will be developed based on its physics and semiconductor properties.
- 2- Modelling the current conduction using Schottky barrier modulation and the tunnelling mechanism in MATLAB.
- 3- Modelling the effect of continuous variation of the interface traps densities and the ideality factor during BRS using MATLAB.
- 4- Modelling the average ionic drift velocity of the oxygen ions by deriving the electric field equation for the un-doped region for the bi-layered RRAM and using Mott and

Gurney rigid point-ion model and Joule heating effect. This equation accounts for the variation of D by using the electric field of the un-doped region. This modelling step is also to be done using MATLAB.

- 5- Modelling the self-limiting growth of the doped region using MATLAB.
- 6- After the initial MATLAB design is implemented and verified, a SPICE model is developed and the simulation results are verified using LTSPICE.
- 7- Modelling the current conduction and the RS behaviour of the Ta/TaO_x/Pt MIM RRAM based on an existing analytical model. The modelling step is done using LTSPICE.

1.6.2. Model Validation and Evaluation Steps

The validity of the bi-layered RRAM SPICE model is verified using three different sets of experimental data from Pt/Ta₂O₅/TaO_x/Pt RRAM with switching layer thickness smaller than 5 nm. The SPICE model should successfully demonstrate four intrinsic features extracted from the experimental observations in which the first three features are related directly to the change in D .

- 1- The bi-layered RRAM SPICE model is first verified that it can produce the correct $I-V$ behaviour when D is changed from 4 to 3 nm.
- 2- The model proves that it can demonstrate the dependency of the high resistance state switching voltage (HSV) on D where HSV is the required voltage for the device to switch into HRS.

- 3- The ability of the SPICE model to demonstrate the effect of changing D on its LRS and HRS is also explored.
- 4- The model is examined and verified that it can successfully capture the temporal increase in the HRS during SET switching.
- 5- Pulse switching simulation with different RESET pulse amplitudes is conducted and the obtained results show that the model can demonstrate the change in the current with regards to RESET pulse amplitude.
- 6- The SPICE model is also tested to show a stable behaviour for its HRS and LRS regions under different types of input signals.
- 7- The integration capability of the proposed SPICE model with the CMOS technology is tested by simulating a non-volatile D-Latch circuit.

PRELIMINARIES ON THE MEMRISTOR / RRAM DEVICES

2.1. The First fabricated Memristor (HP Labs Memristor) and its Operating Mechanism

In general, there are three fundamental electronic circuit elements: the resistor, the inductor and the capacitor. In 1971, Leon Chua argued that there is another missing fundamental element and he called it the memristor (memory resistor) [38].

Chua based his assumption about the memristor on the following analysis. The pairs of the four basic electronic circuit variables (current, voltage, charge, and magnetic flux) are related to each other by six different mathematical equations as can be seen in Figure 2.1. The first equation states that the charge is the time integral of the current. This relation can be found from the definition of the two variables (charge and current). The second equation which is derived from Faraday's law of induction states that the flux is the time integral of the voltage. Therefore, Chua argued that there should be four basic circuit elements which are described by

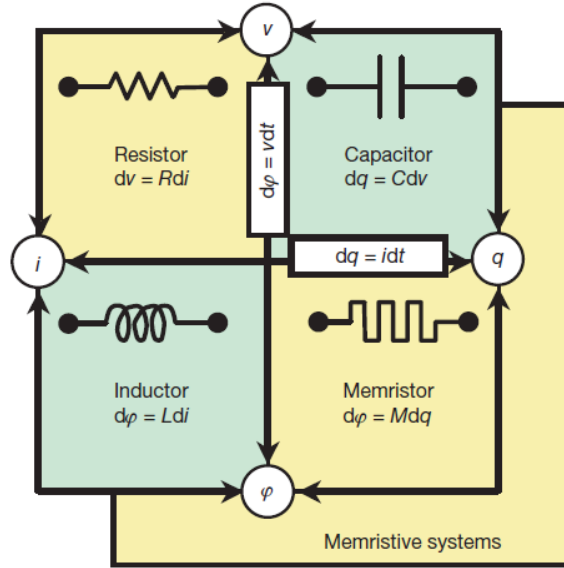


Figure 2.1. The four two-terminal fundamental circuit elements and their related six equations [9].

the remaining four equations between the circuit variable and the memristor is one of these four elements [9]. These six equations and their related elements are shown in Figure 2.1. In Figure 2.1, it is clear that the only missing circuit element is the one between the two variables, the charge and the flux. This missing element is the memristor. The memristor is a two terminal nonlinear circuit element with a memristance M that relates the charge and the flux according to the following equation:

$$d\phi = M dq \quad (1)$$

where ϕ is the magnetic flux and q is the electric charge.

The value of M is not constant but a function of the charge q . This results in a nonlinear relation between the charge and the flux. The I – V characteristic of this nonlinear memristor under

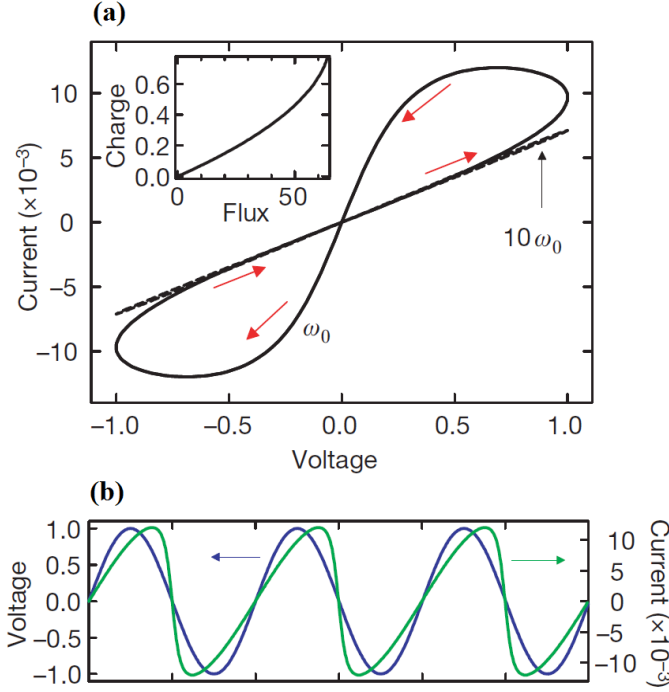


Figure 2.2. (a) The memristor I - V characteristics loops for two different frequencies where the hysteresis loop collapses when the sweep frequency is increased. (b) The memristor applied sinusoidal voltage $v_0 \sin(\omega_0 t)$ (in blue) and the resulting current (in green) as a function of time for the memristor device in [9] where v_0 is the magnitude of the applied voltage and ω_0 is the frequency [9].

sinusoidal input signal is similar to Lissajous figures with a frequency dependent property as shown in Figure 2.2(a). Figure 2.2(a) shows the ideal I - V characteristic loops of the MIM memristor as reported by HP in [9] for two different frequencies where the hysteresis loop collapses when the sweep frequency is increased. Figure 2.2(b) shows the applied input signal to the two terminal memristor device together with the resulted current [9]. However, there is no combination of any nonlinear basic circuit elements which can reproduce the circuit behaviour of the memristor. Since the memristor has this nonlinear behaviour, it can be used in the integrated circuits to provide a unique function such as resistance switching with high densities devices [9].

Until 2008, Chua's idea about the memristor has not been explored and no physical model has been fabricated to show the actual operation of the memristor. However, in 2008, a research group from HP labs announced for the first time that the memristor element exists naturally in the nanometer scale electronic systems where both the ionic conduction mechanism and the solid state electronic are used (under external bias) to describe the memristor equations [9].

The first memristor cell structure announced by HP labs consists of two layers of TiO_2 sandwiched between two platinum electrodes. A schematic diagram of this memristor is shown in Figure 2.3. The first layer is highly doped with oxygen vacancies (behave as a semiconductor) while the second one is an un-doped layer with a higher resistivity (behave as an insulator layer). In Figure 2.3, D is the total length of the oxide layer and w is the length of the doped region. However, depending on the amount of the electric charge flowing in the cell (under an external applied stimulus voltage V), the boundary between the two regions in Figure 2.3 is moving in the same direction of the passing current I [9]. This movement is caused by the oxygen ions/vacancies movement. The flow of mobile dopants increases and decreases the state variable width w of the doped region. Therefore, the resulted memristor total resistance equals to the sum of the series resistances of the doped and undoped regions and is given by [9]:

$$V = \left(R_{\text{ON}} \frac{w}{D} + R_{\text{OFF}} \left(1 - \frac{w}{D} \right) \right) I \quad (2)$$

where R_{ON} and R_{OFF} are the resistances of the semiconductor layer for the memristor when $w = 1$ and 0 , respectively.

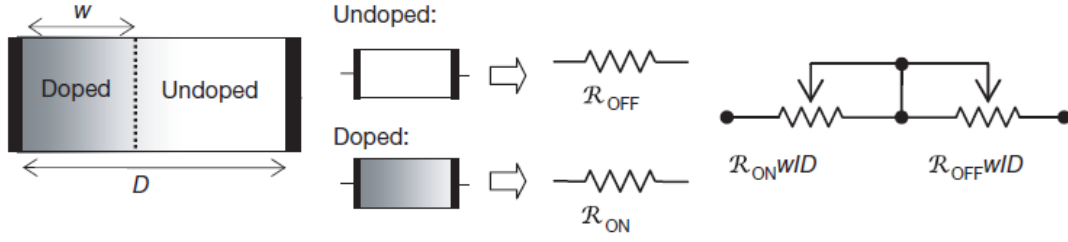


Figure 2.3. A simple equivalent circuit of the variable-resistor model of HP memristor [9].

If the simple case of ionic electronic conduction and linear ionic drift in a uniform field with average ions mobility of μ_V is assumed as in [9], then:

$$\frac{dw}{dt} = \mu_V \frac{R_{ON}}{D} I \quad (3)$$

where μ_V is the average carriers (oxygen vacancies) mobility. Equations (2) and (3) reflect the nonlinear relationship between the integrals of the voltage and current.

However, the memristance is more significant for the electronic devices in nanoscale dimensions [9]. From (3), the value of w is:

$$w = \mu_V \frac{R_{ON}}{D} q \quad (4)$$

Substituting this into (2) and for $R_{ON} \ll R_{OFF}$, we get the values of the memristance $M(q)$ as:

$$M(q) = R_{OFF} \left(1 - \mu_V \frac{R_{ON}}{D^2} q \right) \quad (5)$$

From (5), it clear that the main contribution to the values of memristance $M(q)$ is from the second term in the parentheses. This term increase by decreasing the width of the oxide layer thickness D . As an example, the memristance values would be influenced by this term million

time more significantly when switching from microscale to nanoscale dimensions. This comparison reflects the fact that the memristor does not have a noticeable effect in the micrometre scale devices while in nanometre scale it has a much greater influence on the electronic circuit devices [9]. This is the reason for the memristor being uncovered during the last three decades. However, in order to understand the RS mechanism of the memristor, hereafter will be referred to as RRAM devices, it is essential to understand how the RRAM device is formed prior to the RS mechanism.

2.2. Pre-Resistive Switching Process (Electroforming Process) and the Resistive Switching Mechanism of the MIM RRAM Devices

The metal oxides electrical switching mechanism depends on the coupled motion of the ions and electrons in the oxide material [39]. This electrical switching behaviour is considered as one of the first examples of the memristor/RRAM which was predicted by Chua in 1971 [39]. However, the RRAM devices need an irreversible one step (electroforming) process prior to this electrical switching process. The ideal irreversible electroforming step and the reversible RS behaviour of the RRAM devices are shown in Figure 2.4 [39]. The inset of Figure 2.4 shows the typical MIM RRAM device structure of Si/SiO_x/Ti 5 nm/Pt 15 nm/TiO₂ 25–50 nm/Pt 30 nm.

Before the ON/OFF switching states, the device is in its virgin (almost insulator) state. The repeatable ON/OFF switching states shown in Figure 2.4 can be reached after the electroforming process is applied; by applying a high negative voltage (shown in green colour

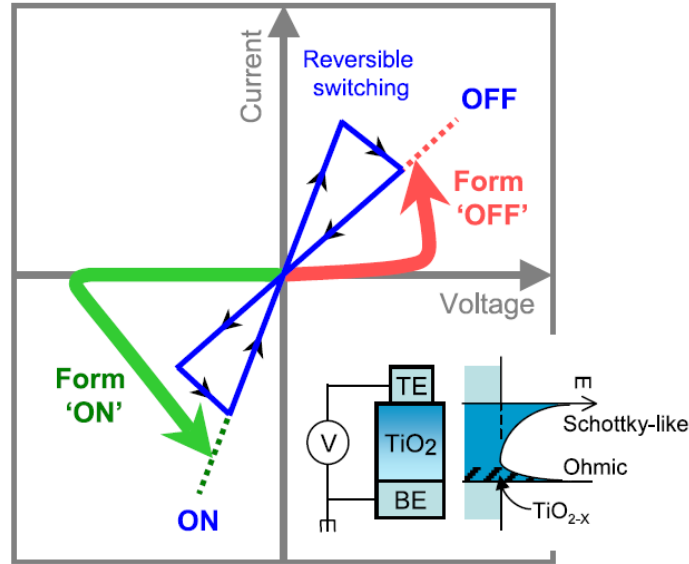


Figure 2.4. The ideal reversible BRS process and the required forming voltage polarity [39].

in Figure 2.4) or high positive voltage (shown in red colour in Figure 2.4). At the electroforming voltage, the device characteristics will change abruptly to a Higher/Lower current and Lower/Higher voltage for negative and positive forming voltages, respectively. The abrupt change in the current indicates the occurrence of the forming and a decrease in the resistance of the device (several orders in the magnitude). After electroforming process, the initial switching state depends on the polarity of the voltage of the electroforming state. The device can then be switched ON and OFF by applying a negative and positive voltages on the TE, respectively. These switching polarities depend on the asymmetry of the interfaces after the device fabrication. In the device shown in Figure 2.4, the top interface is Schottky-like interface while the bottom interface is ohmic [39].

The physics behind the electroforming process can be explained as follows.

The electroforming process in insulator oxides changes the conductivity properties of the insulator (change the behaviour) by applying a high voltage or current (and can be enhanced by electrical Joule heating effect). This high field results in an electro-reduction process together with a vacancy creation in the oxide. The oxygen vacancies are formed and then drift to the cathode (the negatively charged electrode), doping the semiconducting TiO_2 oxide to high conductivities and forming a localized conducting channel through the oxide layer [39]. At the same time, the oxygen ions (O_2^-) will drift to the anode (the positively charge electrode) and change into oxygen gas. Subsequent to this one-time step, the device will operate in its RS (ON/OFF) mode. The oxygen gas formed at the anode could cause a physical deformation in the junctions which in turn results in large variance in the properties of the final device. Therefore, it is highly desirable to eliminate the electroforming process completely. This problem can be reduced by switching the junction area size and the oxide layer thickness into nanometer scale and controlling the polarity of the electroforming process. Engineering the device structure can result in an interface controlled electronics switching which replaces the bulk oxide effect and hence avoid the need for the electroforming process [39].

2.3. The Effect of the Device Area on the Produced Gas Bubbles and The Physical Deformation

The physical deformation problem is related to the area size of the junction of the RRAM device. In [39], two RRAM samples with $5\text{ }\mu\text{m} \times 5\text{ }\mu\text{m}$ micro junction and $50\text{ nm} \times 50\text{ nm}$ nano junction are formed. The oxide layer TiO_2 thickness is the same for both cells, in the range

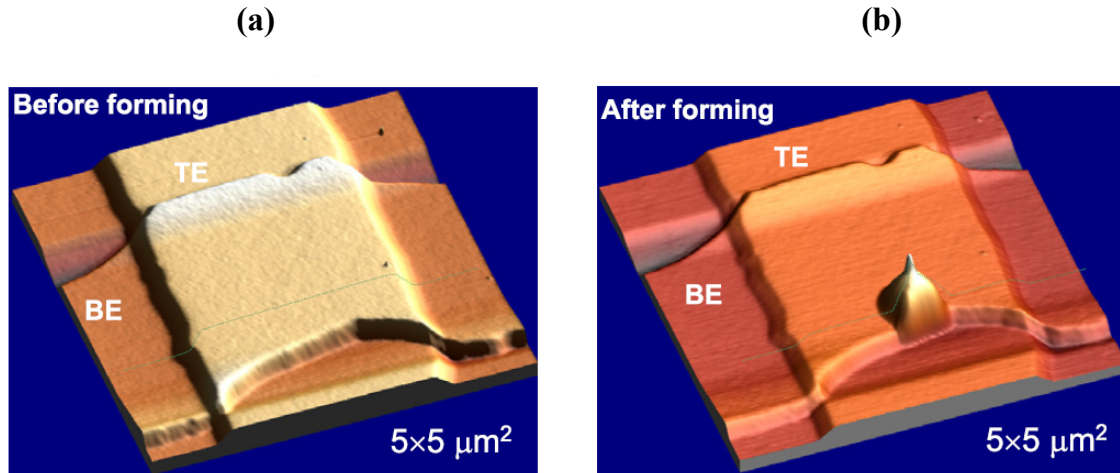


Figure 2.5. (a) Atomic force micrograph (AFM) image of the $5 \times 5 \mu\text{m}^2$ RRAM junction before the electroforming process. (b) AFM image of the same the $5 \times 5 \mu\text{m}^2$ RRAM junction but after applying the electroforming negative voltage. The image shows the bubble formed along the edge of the bottom electrode of the micro scale junction and the pointed tip at the top of this bubble suggests a gap eruption [39].

of 25–50 nm. After the electroforming process, electrical switching performed on them where all the measurements are done by grounding the bottom electrode (BE) and the voltage is connected to the top electrode (TE).

No physical deformation appeared in the nano devices whereas in micro devices a clear and relatively large dome-like appeared beside the edge of the BE. This dome-like deformations is shown in Figure 2.5(b). It can be seen that on the top of this dome there is an eruption-like feature. The assumption is that this deformation is the result of the drift of the negatively charged oxygen ions to the positive electrode. These ions are discharged at that electrode to O_2 gas which, after reaching a certain pressure, finds the mechanically weakest point of the film and erupt from there to form these dome-like phenomena.

As the nano TiO_2 films devices are much smaller in linear dimensions and in volume compared to the micro devices, the amount of the produced material, gas and pressure is much smaller.

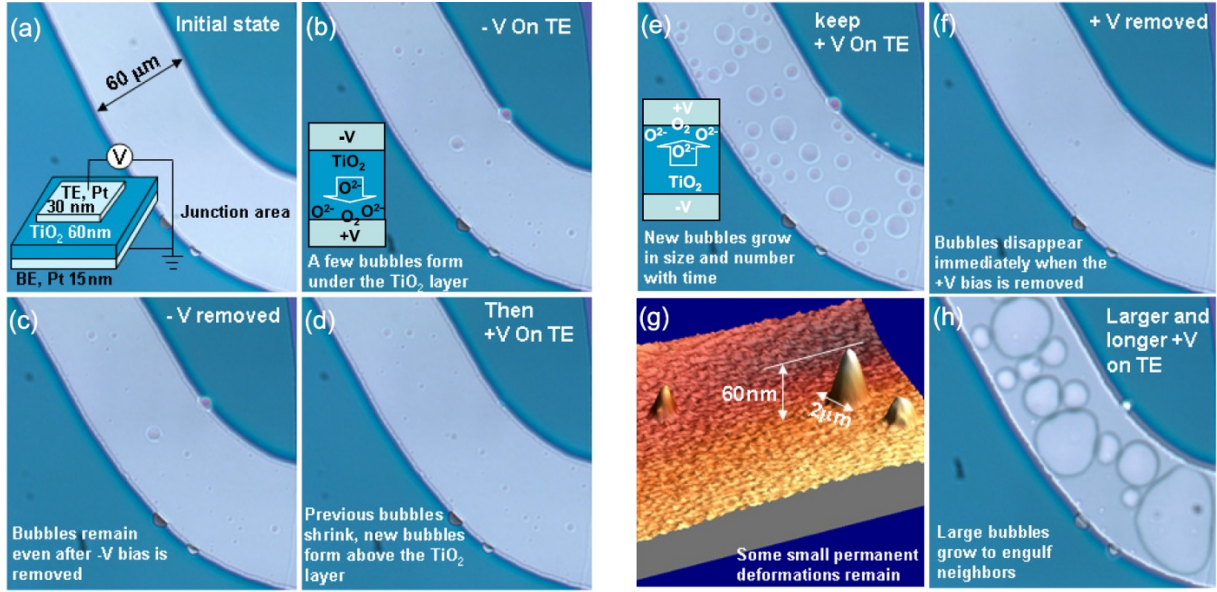


Figure 2.6. The behaviour of the gas bubbles during electroforming process and under different bias polarities. (a) At the initial state (before a bias is applied). (b) and (c) When a negative bias is applied on TE and then removed. (d)–(f) and (h) When a positive bias is applied on TE, keeping the bias for longer time, and then removing the positive bias. (g) AFM image of the eruption feature after removing the positive bias voltage [39].

Therefore, the speed of gas escaping at the oxide film edges is considerably faster for nano films. This explains the improvements in the performance of the switching of the nano over the micro oxide films. As the junction area increased, larger gas bubbles are produced. This is because the gas speed to the electrode's edge in this case is slower than before. As a result of less physical disruption, the nano-device shows better reproducibility than that of the micro-device. This means that the voltage and current variance are lower in the first case [39].

Another important observation of the electroforming process is that when forming the device to ON state (by applying a -4 V on the TE), only few bubbles are produced under the oxide layer [see Figure 2.6(b)] and these bubbles remain even after removing the applied forming voltage [see Figure 2.6(c)]. However, a positive applied voltage of +4 V on the TE would

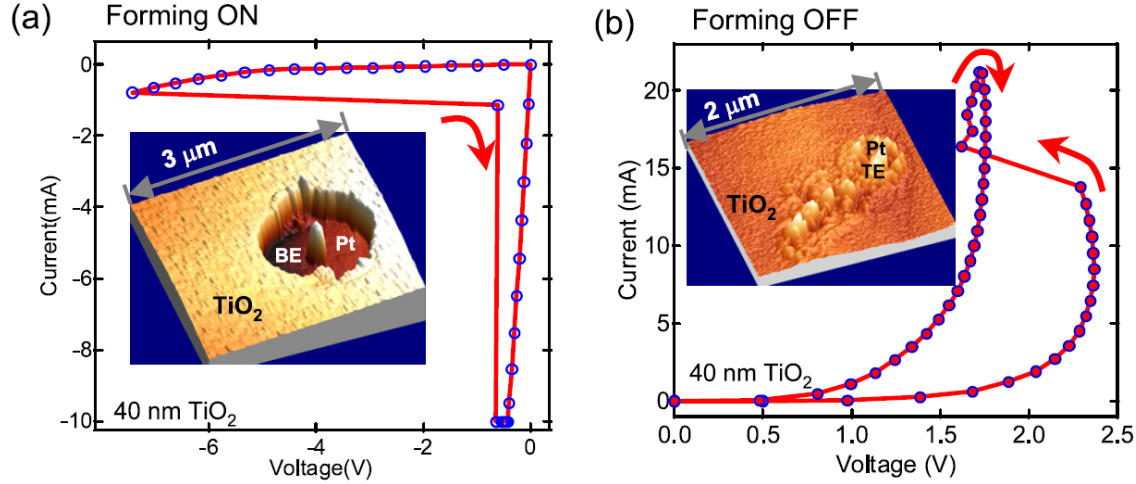


Figure 2.7. Electroforming dependency of the applied bias polarity on the TE (a) Forming the RRAM device into ON state with negative bias. (b) Forming the RRAM device into OFF state with positive bias [39]. The insets in (a) and (b) show the deformation in the RRAM cell after electroforming for both, negative and positive bias polarities, respectively [39].

remove any bubbles under the TiO_2 layer and produces more bubbles above this layer and below the TE layer [see Figure 2.6(d) and (e)]. Increasing the applied voltage would make the bubbles merge with each other and producing larger bubbles. Once the positive applied voltage is removed; all the gas bubbles are disappeared in a few seconds [see Figure 2.6(h) and (f)].

These observations are explained as follow [39]: In the first case (negative bias on TE), the number of gas bubbles is fewer because forming a bubble under the two layers of TiO_2 and TE required more gas pressure than forming the bubbles under only TE layer. Also, the bubbles in the case of the negative voltage don't disappear until a positive is applied on the TE which causes an electrochemical action that reincorporates the gas back to the film. However, in the case of the bubbles formed above the TiO_2 layer (positive bias on TE), they can easily escape through the edges of the electrodes or through an eruption features through the TE [39].

2.4. The Effect of the Asymmetry of the Metal/Oxide interfaces on the Forming Voltage

During the electroforming process, the asymmetry of the two metal/oxide interfaces play a major role in determining the voltage level (the electric field strength) required for the device forming. Figure 2.7 [39] shows the MIM RRAM two devices (with 40 nm TiO_2) are being formed by a negative bias [Figure 2.7(a)] and positive bias [Figure 2.7(b)] to reach the ON and OFF final states, respectively. It can be seen that the average electric field required to form the device to OFF state (+2.3 V) is much smaller (a round one third) compared to the electric field required to form the device to the ON state (-7.8 V) [39]. This can be explained by knowing that the Schottky-like interface between the TE and the oxide TiO_2 layer is forward biased during the forming/switching to the OFF state (positive bias on the TE). Therefore, the current is higher during this switching stage compared to forming/switching the device to ON state with a negative bias (reversed biased Schottky barrier). Hence, the possibility of Joule heating effect is high (the temperature can reach several hundred degrees in this case [39]). Due to the high temperature, oxygen vacancies mobility can increase by around seven order of magnitude at 240 $^{\circ}\text{C}$ compared to the mobility at room temperature [39]. This shows that the electroforming process is first triggered by the applied electric field and then enhanced by the electrical heating (the oxygen ions/vacancies are created at the region of the high electric field and then drift into the positive/negative electrode [39]).

2.5. Overall Summary of the Electroforming Step

2.5.1. Electroforming the RRAM Device into ON Initial State

- 1- Electroforming by negative voltage on the TE results in an initial ON state (SET).
- 2- During SET electroforming, the negative voltage on TE results in a large voltage drop on the reverse-biased Schottky-like interface. The oxygen vacancies will be generated at the interface region and stay there until their doping effect reduces the electronic barrier into conductive and the electric field at that area will drop [39].
- 3- The current increases but will be limited by the insulating bulk layer which is considered now as the high electric field region of the RRAM device [39].
- 4- As more oxygen vacancies are created and drift across the bulk layer to create a CF, the resistive Schottky-like interface and the resistive bulk layer will both be penetrated by a conducting channel and the RRAM device reaches its LRS (ON state).
- 5- The inset of Figure 2.7(a) shows the device after removing the TE. It can be seen that a round hole is formed in the oxide layer, indicating that the oxygen gas bubbles are likely formed under the oxide layer.

2.5.2. Electroforming the RRAM Device into OFF Initial State

- 1- Electroforming by positive voltage on the TE results in an initial OFF state (RESET).
- 2- During this stage, the forward-biased Schottky-like interface will be relatively conductive. Hence, the voltage drop will be concentrated on the bulk layer [39].

- 3- Oxygen ions will drift toward TE and discharge there to form oxygen gas on the top of the oxide layer and below TE. At the same time, oxygen vacancies will drift away from the top interface, toward BE which form CF through the oxide film [39].
- 4- However, due to the polarity of the electric field in this case (positive voltage on TE), the electric field will repel away the vacancy channels from touching the TE and hence, Schottky-like interface will not be heavily doped by the oxygen vacancies and the initial state after forming is OFF state. According to [39], the CF penetrates the bulk layer but it doesn't do the same at Schottky-like interface region.
- 5- The inset of Figure 2.7(b) shows that the oxide layer is less physically deformed by the produced gas bubbles when compared to electroforming by negative bias (because the gas bubbles were formed on top of the oxide layer and under TE). The deformation has mainly affected the TE/oxide layer interface.
- 6- According to [39], the bubbles are formed in the centre of the junction area and the position of the conducting channels is adjacent to the bubble area.

LITERATURE REVIEW ON THE MIM AND MISM RRAM MODELS

Summary

Several RRAM models have been presented in the literatures. These models can be divided into MIM RRAM models and MISM (bi-layered) RRAM models. In this chapter, a literature review on both types of RRAM models will be conducted to further explain why the available models cannot be used directly to reproduce the behaviour of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM devices.

3.1. MIM Mathematical and SPICE RRAM Models

From the literature, it can be seen that a great progress has been made on the analytical and SPICE modelling of the MIM RRAM devices [15], [40], [41], [42], [43]. Also, evaluation criteria have been introduced in [44] which can be used to check the applicability of these models to simulate the RS behaviour.

Some models aim to have the flexibility to fit into different physical MIM RRAM models [15], [40]. The model in [40] is correlated against several MIM RRAM devices with an average error of 6.04%. It was also tested in a relatively large circuit of 256 RRAM devices and showed better results when compared to the available MIM RRAM devices (caused less convergence errors). In this model, a hyperbolic sinusoid equation of the MIM tunnel barrier for electron tunnelling is used to model the MIM junction conduction which showed the best fit with the experimental data. However, in the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM, the conduction equation is based on Schottky barrier modulation and tunnelling mechanism in the MIS structure. The model in [40] uses fitting parameters to show that the RRAM is more conductive in the positive region than the negative region whereas the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM exhibit this behaviour due to its Schottky barrier being forward biased and reversed biased for positive and negative bias, respectively, which should be taken into account when developing a $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM model.

The state variable in [40] is based on two mathematical functions: the first function accounts for the threshold voltage required for the state change. This function uses fitting parameters to determine how quickly the state change once the threshold voltage is reached. Although this function can provide different threshold voltages based on the bias polarity, it doesn't reflect the physics involved in the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM devices. The state variable in [40] does not take into consideration the ions hopping mechanisms in the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM which is the responsible mechanism for the change in the resistance during the RS process and can be modelled using the ions hopping hyperbolic sinusoidal programming

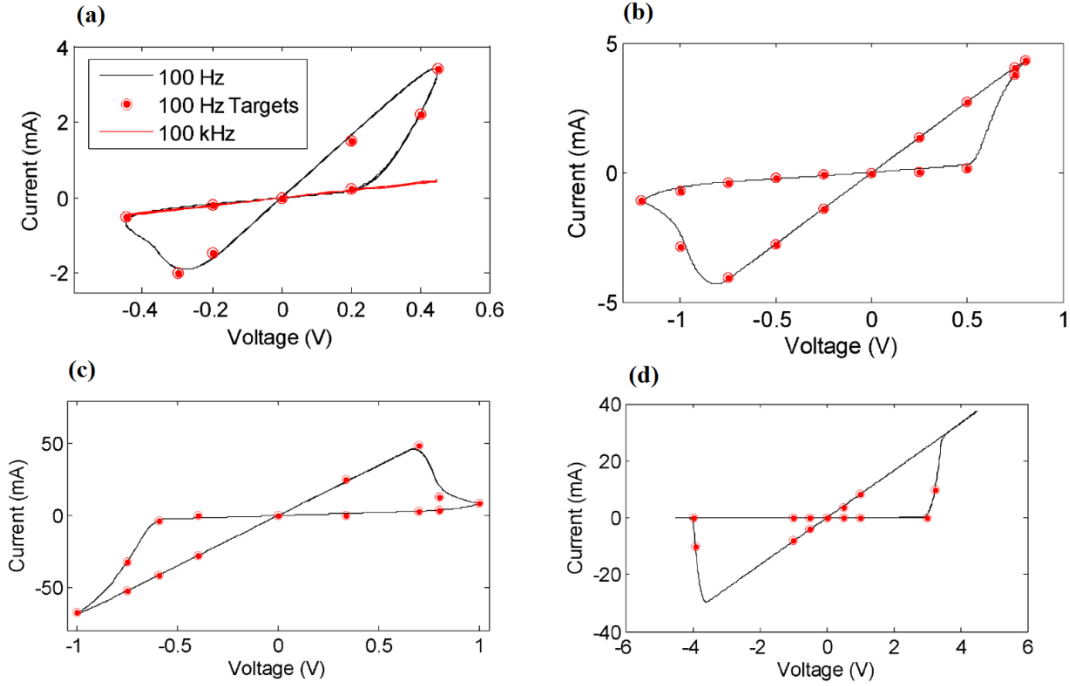


Figure 3.1. The simulation results of the RRAM physical devices in (a) [45], (b) [46], (c) [47] and [48], and (d) [49] modelled using the MIM RRAM model proposed in [40].

threshold (Mott and Gurney rigid point-ion model) and Joule heating effect. It also does not consider the electric field effect in the ions hopping region which determines the threshold voltage and should be incorporated in the bi-layered RRAM mathematical model. The second function in [40] models the nonlinear dopant drift based on the bias polarity.

Figure 3.1(a)–(d) shows the MIM RRAM devices in [45], [46], [47], [48], and [49] modelled using the MIM RRAM model in [40]. The simulation results in Figure 3.1(a) match with the experimental data in [45] with an average error of 6.64%. Figure 3.1(b) shows the simulation results of the RRAM device in [46], modelled using the RRAM SPICE model in [40] with an average error of 6.21%. Figure 3.1(c) shows the simulated I – V curves from the RRAM devices in [47] and [48] which matches to the experimental data with an average error of 5.97%. As a

final example for using the SPICE model in [40] to model MIM RRAM devices, Figure 3.1(d) depicts the simulation results of modelling the physical RRAM device in [49] with an average error of 6.15%. Although the MIM RRAM model in [40] showed good agreements with the experimental results for different MIM RRAM devices, it can be seen in Figure 3.1 that all these RRAM devices showed different characteristics when compared to the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM. Hence, the SPICE model in [40] cannot be applied directly to the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM.

Another MIM RRAM model is presented in [15] and proved that it can fit into several MIM RRAM devices with reasonable accuracy, computational efficiency, and with mean error of 0.2%. The $I-V$ relationship in this model is not defined and claimed that it can be chosen from any of the available $I-V$ conduction relationships. The expression of the derivative of the state variable of the model in [15] (which also represents the RS speed) is claimed to have the flexibility to fit into any RRAM device type. However, this expression does not take the intrinsic Schottky-like interface, Joule heating effect, ions hopping mechanism and the electric field dependence of the growth rate equation into consideration. Therefore, similar to the model in [40], this model cannot be applied directly to the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM devices which exhibit different characteristics when compared to the model in [15].

Some models have been proposed to model the TaO_x -based MIM and bi-layered RRAM devices as in [41]. In [41], a circuit-based model for TaO_x -based MIM RRAM RS is presented and implemented in VerilogA. The model is designed to match the behaviour of $\text{Pt}/\text{TaO}_x/\text{Ta}$ MIM RRAM device with the TaO_x thickness of 11 nm and the obtained simulation results were

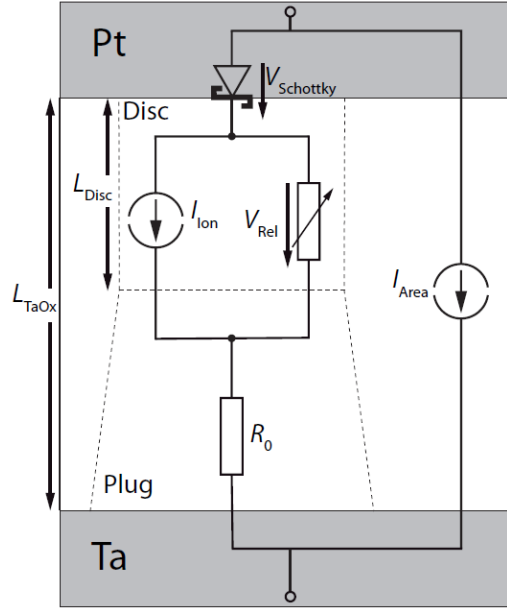


Figure 3.2. The Equivalent circuit model and the cell structure of the Pt/TaO_x/Ta MIM RRAM model in [41].

compared to the experimental results taken from [50]. This model is one of the best physical-oriented TaO_x-based RRAM models which takes into consideration Schottky-like interface between the TE and the oxide layer. It also considers the temperature effect during RS. Furthermore, this model also added the ionic current and the areal current components and used the oxygen vacancies concentration as the state variable which can change the value of the electronic resistance R_{e1} and Schottky barrier height (see Figure 3.2). As can be seen in Figure 3.2, the model consists of a well conducting plug (modelled as a series resistor) and a more resistive switching layer (the disc in Figure 3.2).

However, due to the device thickness (11 nm) in [41], a large area dependent parallel current is presented in the device besides the current through the CF (see Figure 3.2). This areal current

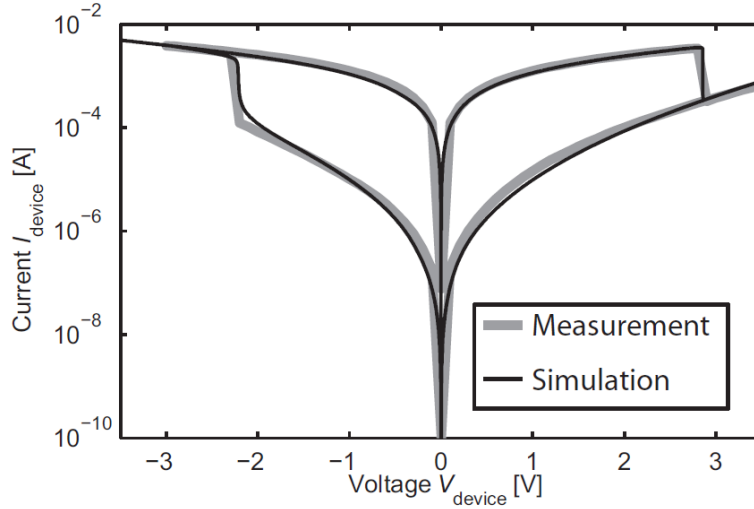


Figure 3.3. The measured I - V characteristics from [50] and the simulation results in [41] for the Pt/TaO_x/Ta MIM RRAM device with TaO_x thickness of 11 nm plotted on logarithmic scale [41].

is the dominant current during HRS. For this areal current, Poole-Frenkel-type conduction mechanism showed good fitting for the 11 nm TaO_x-based MIM RRAM. Besides that, Fowler-Nordheim tunnelling mechanism showed good fitting when used for the negative bias. However, it is expected that the current of the RRAM devices has a great relevance for the oxide thickness (especially at HRS) which implies that different conduction mechanisms exist for RRAM devices with different oxide thickness [32], [50]. For example, Schottky barrier modulation and tunnelling mechanism showed good fitting for the Ta₂O₅/TaO_x bi-layered RRAM with switching layer thickness in the range of 3–4 nm while the conduction mechanism used in [41] (Poole-Frenkel-type conduction and Fowler-Nordheim tunnelling mechanism) did not fit into the same RRAM with oxide thickness 3–4 nm. This behaviour agrees with the physics of these conduction mechanisms, where each current mechanism is valid under certain range of thicknesses only. Therefore, the model in [41] is limited to the devices with a relatively thick oxide layers and cannot be applied directly or modified to fit the Ta₂O₅/TaO_x bi-layered

RRAM device modelled in this research (3–4 nm). Other conduction mechanisms also exist and can be tested for RRAM with oxide layer thickness in the range of 5–10 nm. Example of such mechanisms are direct tunnelling, Fowler-Nordheim tunnelling...etc.

In general, if the design does not follow the correct physics involved in the conduction mechanism, it will fail for operation outside the measured data window.

The state variable and the resistance evolution in [41] are developed based on the oxygen ions concentration in the disc. Therefore, the switching region is assumed to be of a fixed thickness and the electric field is calculated over the entire disc thickness. However, in order to predict the oxygen ion migration mechanism for the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM using Mott and Gurney rigid point-ion model, the electric field in the active switching region for the bi-layered RRAM structure must first be calculated.

For all the above mentioned reasons, the RRAM device model in [41] shows different I – V characteristics when compare to the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM device modelled in this research. Figure 3.3 shows the I – V behaviour of the model in [41] fitted to the physical Pt/ TaO_x /Ta RRAM device with the TaO_x thickness of 11 nm as in [50]. The behaviour of the Pt/ TaO_x /Ta RRAM in figure 3.3 can be compared with the behaviour of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM in figure 4.2, which shows how the characteristics of the two devices are different. Therefore, the RRAM model in [41] cannot be applied directly to simulate the behaviour of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM.

Similar to the above mentioned models, many other MIM RRAM models have been presented and explained in the literatures [42], [43], [51], [52], [53], [54]. While these MIM models are

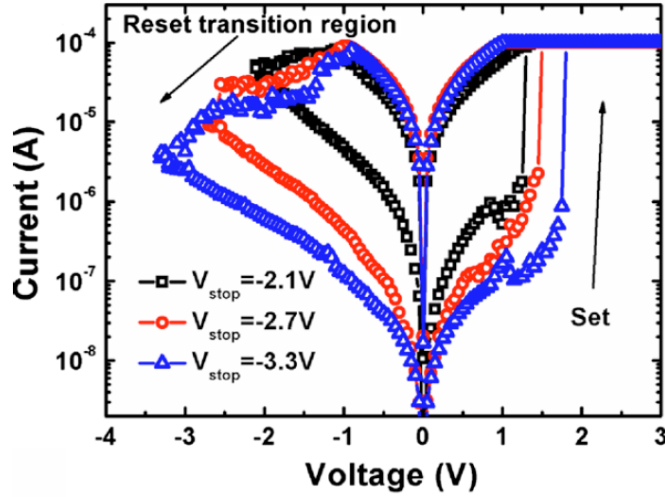


Figure 3.4. The typical I - V characteristics of the HfO_x/AlO_x RRAM measured by DC sweep. Different RESET pulse stops voltages of (-2.1, -2.7, and -3.3 V) were used [24].

computationally efficient and showed good agreement with the measured data, the physics behind the behaviour of the Ta₂O₅/TaO_x bi-layered RRAM has not been fully covered or explained in these models. Therefore, a solid, physics-based Ta₂O₅/TaO_x bi-layered RRAM model is still missing in the literature.

3.2. Bi-layered RRAM ANALYTICAL AND SPICE Models

Besides the MIM RRAM models, few analytical models: AlO_x/WO_x [22], HfO_x/AlO_x [24] and [25], and SPICE models: TiO_x/HfO_x [51], Zr/HfO_x [52], and HfO_x/AlO_x [53], have been developed to reproduce the behaviour of some bi-layered RRAM devices for different oxide material and different oxide layer thickness. However, each of these models showed different characteristics based on the oxide material of the device they designed to match. Therefore, they cannot be applied directly to the Ta₂O₅/TaO_x bi-layered RRAM devices. This limitation

is attributed to the physics behind the behaviour of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM which has not been fully covered in these models. Some of these bi-layered RRAM models are explained in the following discussion.

Modelling of $\text{HfO}_x/\text{AlO}_x$ RRAM is demonstrated in [24], and [25]. In [24], a RS RRAM model of $\text{TiN}/\text{HfO}_x/\text{AlO}_x/\text{Pt}$ thin film is proposed. The typical I – V characteristics of the $\text{HfO}_x/\text{AlO}_x$ RRAM is shown in Figure 3.4 which is obtained by applying different RESET stop voltages. In [24], the voltage drops on Schottky barrier contact and the bulk layer are not considered in the oxygen ions drift equation which means that this model cannot be used directly to model the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM. Although this model takes into account the ions hopping

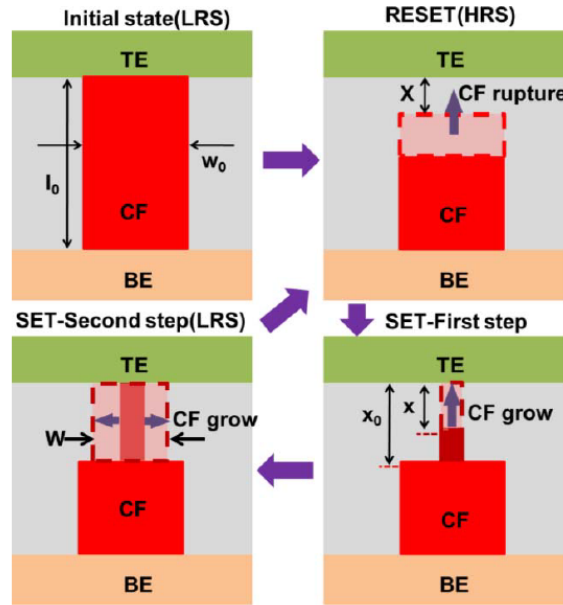


Figure 3.5. 3-D Evolution dynamics of the SET and RESET process of the model in [25].

process through the oxide material and the electric field in the switching region, the model in [24] is mainly utilized to elucidate the RS evolution in the RESET process without modelling the current conduction. Besides the lack of the current conduction modelling, the $\text{HfO}_x/\text{AlO}_x$ RRAM shows different characteristics when compared to the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM devices (compare Figure 3.4 with the I - V behaviour of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM in Figure 3.11(b)).

In [25], a physics-based $\text{HfO}_x/\text{AlO}_x$ bi-layered RRAM model is proposed. The results of the simulated I - V curve and its corresponding CF geometry evolution show that the RESET process is corresponding to CF disconnecting first at the TE and then extending toward the interior as the voltage increases. The SET process on the other hand is corresponding to the

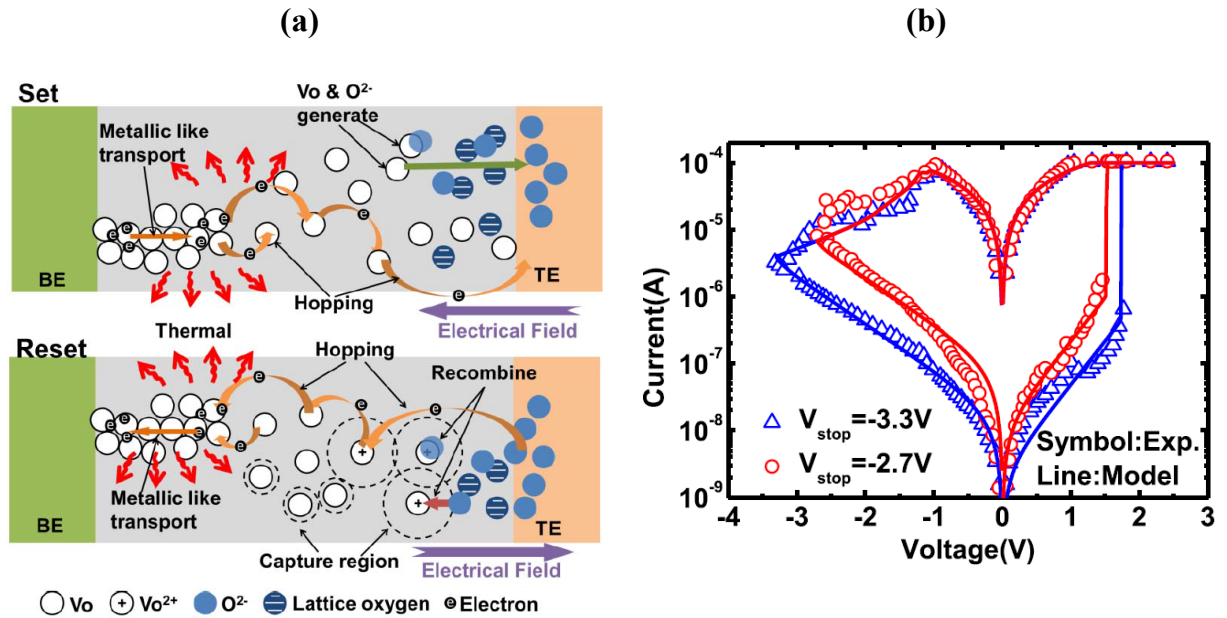


Figure 3.6. (a) The current conduction mechanism in the CF and the gap regions of the model in [25]. (b) The simulation results and the measured data of $\text{TiN}/\text{HfO}_x/\text{AlO}_x/\text{Pt}$ bi-layered RRAM from [24] obtained by dc double sweep [25].

formation of a fine CF in the rupture region which first connect the TE with the tip of the CF. Then, the CF gradually enlarging along the radius direction as the current increases. The 3-D evolution of this process is shown in Figure 3.5 [25]. However, the RS mechanism in the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM is based on vertical growth and rupture evolution mechanism only which is different from the model in [25].

As can be seen in Figure 3.6(a), the current conduction mechanism in this model is based on the metallic-like conduction (in the CF region) and the hopping conduction (the conduction of the gap region) which is different from the Schottky barrier modulation and tunnelling current used for the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ RRAM [1], [8], [21]. The simulation result obtained in [25] is compared with the measured data of $\text{TiN}/\text{HfO}_x/\text{AlO}_x/\text{Pt}$ bi-layered RRAM from [24]. The

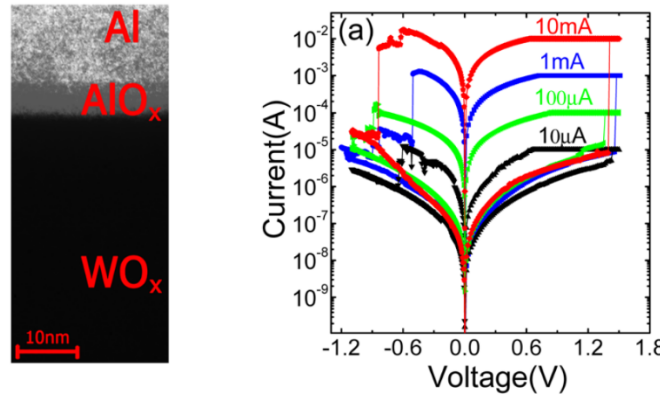


Figure 3.7. (a) Cross-sectional field-emission TEM of the AlO_x/WO_x bi-layered RRAM device in [22]. (b) I - V characteristics of different resistance state achieved by applying four different RESET voltages [22].

measured and the fitting I - V simulation results are shown in Figure 3.6(b) obtained under DC sweep mode. It can be found that the RS behaviour is different from the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM (see Figure 3.11(b)). The device switches ON and OFF under positive and negatives

voltages, opposite to the voltage switching polarities of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM. Also, it can be seen that the SET voltage is smaller than RESET voltage, which is also different from the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM devices, where a higher SET voltage is required to switch the device to its ON state. Furthermore, the switching regions behaviour are also different for the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM devices. This further prove that this model cannot be applied directly to the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM. Finally, this model has not been implemented in SPICE and hence, it cannot be used directly in the RRAM-based circuit applications.

The conduction in AlO_x/WO_x bi-layered RRAM is investigated in [22] where a model of the $\text{Al}/\text{AlO}_x/\text{WO}_x/\text{W}$ bi-layered RRAM structure is presented. After fabricating the device, a 6 nm thick AlO_x layer is clearly observed between the Al and WO_x layers where the AlO_x acts as the

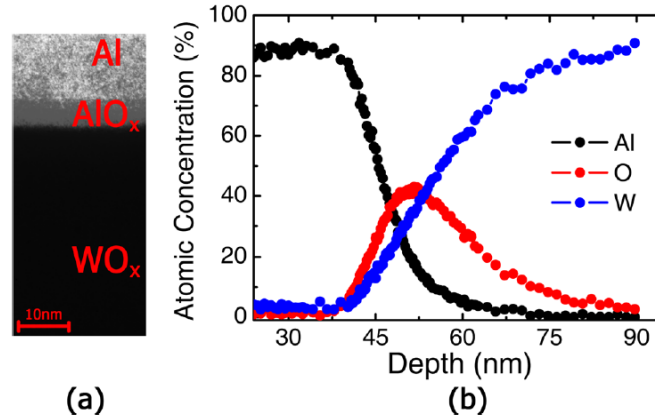


Figure 3.8. (a) Cross-sectional TEM image of the RRAM device in [22]. (b) AES depth analysis of the bi-layered RRAM in [22].

RS layer in this RRAM device. The cross-sectional field-emission TEM of this RRAM device is shown in Figure 3.7(a) while Figure 3.7(b) shows the I - V characteristics of different

resistance state achieved by applying four different RESET voltages. The first imperative remark that can be observed in Figure 3.7 is that the device shows opposite switching polarity when compared to the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM where SET process occurs when a positive bias is applied on the TE. This behaviour can be explained as follows.

Figure 3.8(b) shows the AES depth analysis which confirms the existence of W, Al, and O elements in the AlO_x switching layer. This means that this layer could have AlO_x , WO_x (oxygen could form bonds with either Al or W atoms), and free Al and W metals. However, during SET process, the metal-O bonds break and then the oxygen ions diffuse to the top Al electrode (due to the effect of the electric field) [22], which leave metal atoms in the interface layer. The metal atoms form metal CF. According to [22], it is expected that it is easier for the oxygen to break away from W-O bond than from Al-O bonds in the AlO_x layer. This is because the W-O bond is much weaker than Al-O bond (Gibbs energies are -506.63 kJ/mol and -1582.3 kJ/mol for W-O and Al-O bonds, respectively). As a result, W contributes more to the metal filament than Al. However, the RS process in the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM is different, where the CF is formed due to oxygen ions hopping and the doping effect of their corresponding oxygen vacancies, not due to the metal atoms as in the AlO_x/WO_x bi-layered RRAM.

The current conduction mechanism in [22] at HRS is assumed to follow Schottky emission at the Al- AlO_x interface which showed good fitting with the experimental data. The conduction mechanism at LRS is assumed to be ohmic conduction while the conduction between LRS and HRS (medium resistance) is assumed to be electron hopping conduction mechanism. However, Schottky emission model in [22] is different from that in $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM [21]. It does not take into account the possible tunnelling, the effect of the continuous variation of the interface traps, and the image force lowering [32]. The image force is an induced charge on

the metal electrode surface due to the presence of an electron/hole on the semiconductor interface. This charge is equal to the carrier charge at the semiconductor but with opposite polarity. This leads to the formation of an attraction force between the carrier charge and its image charge, inducing a potential energy on the carriers. The potential associated with the charge carriers together with the potential energy due to the applied field reduce the effective Schottky barrier height [32]. The difference in the conduction mechanism could be attributed to the thicker switching layer in the model in [22] (6 nm) when compared to that of the Ta₂O₅/TaO_x RRAM (3 and 4 nm) [32], [50]. It can also be attributed to the difference in the switching interface material (Al-AlO_x for the model in [22] and Pt-Ta₂O₅ for the model in this research). In addition to the difference in the conduction mechanism, the model [22] does not model the RS dynamic behaviour.

In addition to these bi-layered RRAM models, several analytical and physical Ta₂O₅/TaO_x bi-layered RRAM models have been illustrated in the literature [1], [8], [16], [17], [18], [19], [20], [21], and some of these models have been explained in [21]. However, to the best of the researcher knowledge, these models have not been automated through a computer aided design tool and the SPICE model to predict the Ta₂O₅/TaO_x bi-layered RRAM device behaviour in the circuit level is not yet available.

In [18], an electro-thermal RS model for the Ta₂O₅/TaO_x bi-layered RRAM is presented. The model is based on the temperature and field accelerated migration of oxygen vacancies. The model predicts the temperature inside the doped region and it is one of the best models that investigate the thermal effect of the oxygen ions during RS in the Ta₂O₅/TaO_x RRAM. The RS

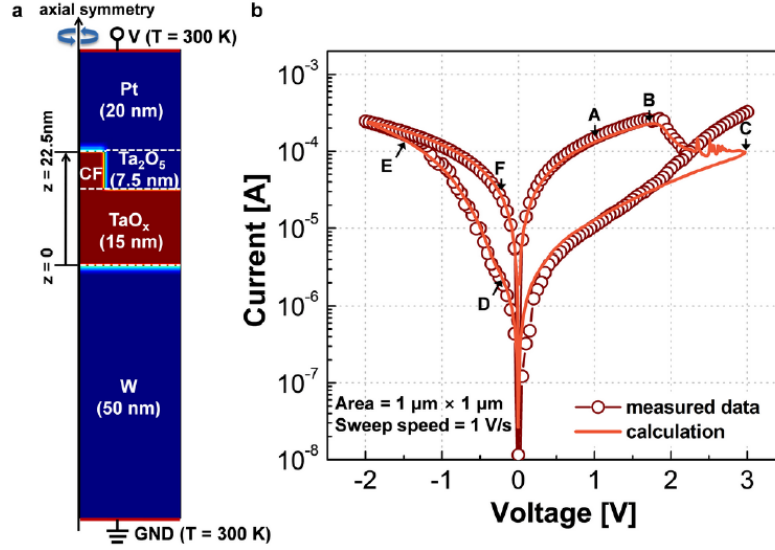


Figure 3.9. (a) Cross section of the bi-layered RRAM cell simulated in [18]. (b) The simulation results and the measured $I-V$ characteristics as reported in [18] for Ta₂O₅ layer thickness of 7.5 nm. [18]

in this model is based on the formation and rupture of the doped region in the insulator layer without considering the intrinsic Schottky-like interface. The current continuity equation for investigate the thermal effect of the oxygen ions during RS in the Ta₂O₅/TaO_x RRAM. The RS in this model is based on the formation and rupture of the doped region in the insulator layer without considering the intrinsic Schottky-like interface. The current continuity equation for electrical conduction showed good fitting with the device $I-V$ characteristics. It can be seen in Figure 3.9(b) that the device behaviour for the Ta₂O₅/TaO_x bi-layered RRAM with Ta₂O₅ layer thickness 7.5 nm is different from the device $I-V$ characteristics for the same bi-layered RRAM structure but with Ta₂O₅ layer thickness smaller than 5 nm [see Figure 3.11(b)]. For example, an abrupt SET switching is observed when Ta₂O₅ layer thickness is smaller than 5 nm [see Figure 3.11(b)] whereas the SET switching in the case of Ta₂O₅ layer thickness of 7.5 nm is

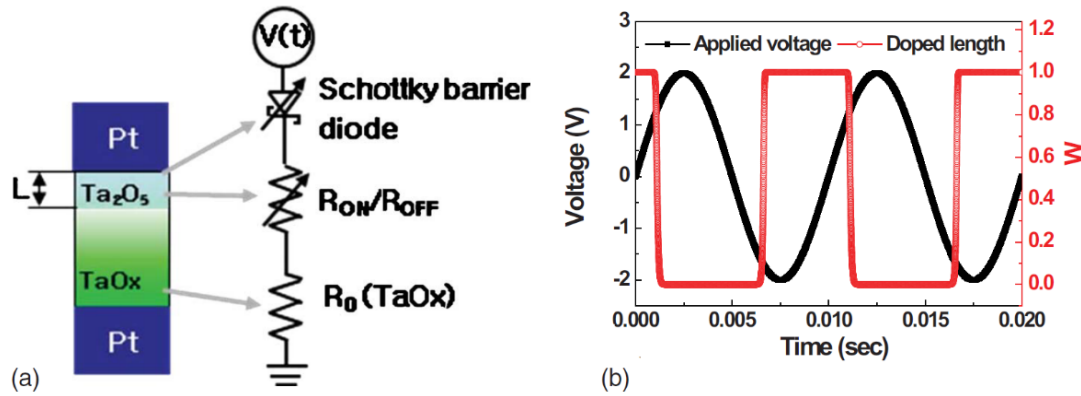


Figure 3.10. (a) The equivalent circuit used in the model in [16]. (b) The doped region thickness w normalized to D in response to a sinewave signal [16].

gradual. The differences in the current conduction mechanism and the I - V characteristics could be attributed to the fact that different current conduction mechanisms exist for RRAM devices with different oxide layer thickness [32], [50]. Therefore, this model cannot be applied directly to the Ta₂O₅/TaO_x bi-layered RRAM of smaller insulator layer (< 5 nm).

Besides [18], among the first developed Ta₂O₅/TaO_x bi-layered RRAM models are presented in [16] and [17]. In [16], a mathematical model that can describe BRS in metal-oxide RRAM for Ta₂O₅/TaO_x bi-layered with Ta₂O₅ layer thickness of 4 nm is presented. The BRS in this RRAM model is explained based on Schottky barrier modulation caused by doping-level variation in the thin oxide layer. The equivalent circuit used in this model is shown on Figure 3.10(a) together with the structure of the cell that correspond to each circuit element. The oxygen-vacancy transport in [16] is obtained by adopting a simplified drift model, similar to that used in the TiO₂-based RRAM. The transport equation does not take into account the ions hopping mechanism responsible for the RS process. Also the effect of the electric field on the

nonlinearity of the oxygen ions drift speed is not considered in [16]. Thus, the oxygen ions/vacancies transport equation does not represent the real physics involved in the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM RS mechanism.

The conduction mechanism in the model in [16] is based on the classical mechanics where only the mobile carriers with energies higher than the barriers energy can escape the potential barrier in the RRAM device [32]. Therefore, the tunnelling current (due to the insulator layer effect) is ignored in this model. However, at room temperature, the presence of the insulator layer in the MIS system has certain effects on the device behaviour. First, it leads to the modification of TPF term which is used to determine the tunnelling current. The value of TPF will depart from 1 (which indicates that the thermionic emission is the conduction process) to significantly smaller values to emphasize the occurrence of tunnelling in the device [32]. In [16], TPF has not been considered by the RRAM current equation. As TPF reduces the memristor current significantly, including it in the current equation becomes vital. Therefore, since the Ta_2O_5 layer thickness in the studied $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM is in the allowable range of tunnelling, the model should be developed based on different approach than the one presented in [16]. It should be developed by incorporating the tunnelling current mechanism. The conduction mechanism in [16] depends on the applied bias to determine the variation in its ideality factor in which the model uses only two discrete values for the interface traps densities and the ideality factor. Hence, the model does not exhibit the actual physical mechanism of the continuous charging and discharging of the interface traps.

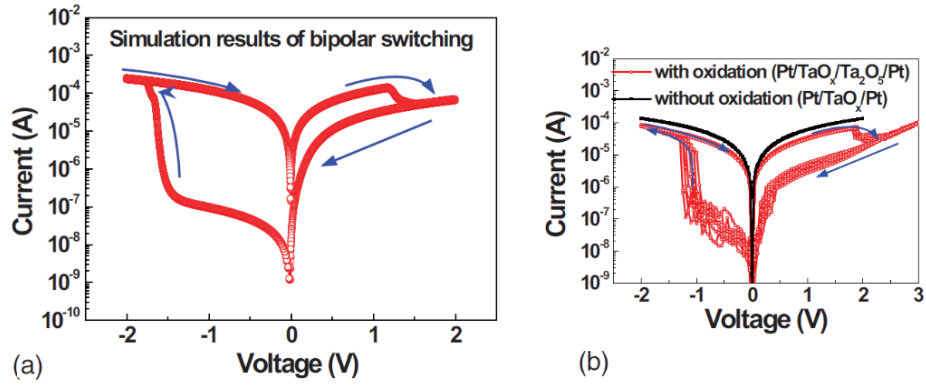


Figure 3.11. (a) The simulation results and (b) the measured data of the model in [16].

Figure 3.10(b) shows the doped region thickness w normalized to D in response to a sinewave signal. It can be seen in this figure that the model is simulated under 2 V RESET bias signal, which is different from the voltage amplitude used in the experiments [3 V RESET bias signal, see Figure 3.10(b)]. This result in a different HSV voltage (≈ 1.3 V) when compared to the experimental results (≈ 1.9 V) (see Figure 3.10). Also, it can be seen in Figure 3.10 that the simulation LRS current is slightly larger than the measured LRS. Although this model showed good agreement with the experimental results, the modelling of the ionic transport mechanism in [16] is highly idealized and the effect of the insulator layer on the conduction process can be further explained when analysed in terms of the semiconductor properties. Also, the Joule heating effect is not considered in [16] and the model has not been implemented in SPICE and hence, cannot be used directly in the RRAM-based circuit applications.

Similar to the model in [16], the model in [17] is also based on the classical mechanics where only the mobile carriers with energies higher than the barriers energy can escape the potential barrier in the RRAM device [32] and TPF is not used in this model. The conduction mechanism

in [17] is using a constant ideality factor. Hence, similar to the RRAM model in [16], the model does not exhibit the actual physical mechanism of the continuous charging and discharging of the interface traps. In addition, Joule heating effect is not considered during the RS process in [17] and the temperature is assumed to be at room temperature. Although the model in [17] showed good agreement with the experimental results, the modelling of the effect of the insulator layer on the conduction process can be further explained when analysed in terms of the semiconductor properties. Most importantly, this model has not been implemented as SPICE subcircuit. Therefore, it cannot be used in RRAM-based circuit applications.

MATHEMATICAL MODELING OF THE Pt/Ta₂O₅/TaO_x/Pt BI-LAYERED RRAM

Related Publications:

F. O. Hatem, P. W. C. Ho, T. N. Kumar, and H. A. F. Almurib, “Modeling of bipolar resistive switching of a nonlinear MISM memristor,” *Semicond. Sci. Technol.*, vol. 30, no. 11, 2015.

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Summary

This chapter presents a deep theoretical discussion of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM and propose a novel and accurate mathematical model of a BRS of the bi-layered $\text{Pt}/\text{Ta}_2\text{O}_5/\text{TaO}_x/\text{Pt}$ RRAM. The proposed model describes the BRS behaviour based on the fundamentals and physical characteristics of the MIS system. It also includes the physical characteristics of the insulator layer. When compared to the existing models with the same cell structure, the novelty of the proposed model lies in incorporating TPF term between the semiconductor and the metal layers and therefore, demonstrating its effect on the conduction mechanism. In addition, the effect of continuous variation of the interface traps densities and the ideality factor during BRS is explained and modelled using the semiconductor properties and the characteristics of the MIS system. Thus, the model emphasizes the dependency of the RRAM current on the physical characteristics of the insulator layer. This overcomes the previous assumption that the interface traps in the MIS RRAM are fixed during the switching time and only changes once the polarity of the RRAM input signal is changed. Moreover, the electric field equation for the active region is derived for the bi-layered RRAM structure which is used together with Mott and Gurney rigid point-ion model and Joule heating effect to model the oxygen ion migration mechanism. Finally, the model also demonstrates the self-limiting growth of the doped region. The modelling steps are introduced in details throughout the chapter sections and the final model is correlated against the experimental results of the published devices which have the same bi-layered RRAM structure and same material. Extensive simulation is carried out on the proposed model which show that the proposed model is in good agreement with the physical characteristics of the $\text{Pt}/\text{Ta}_2\text{O}_5/\text{TaO}_x/\text{Pt}$ RRAM.

4.1. The Structure and the Semiconductor Properties of the Pt/Ta₂O₅/TaO_x/Pt RRAM Proposed Model

4.1.1. The Structure of the Proposed Model

The structure of the oxide-based Pt/Ta₂O₅/TaO_x/Pt RRAM cell modelled in this chapter is shown in Figure 4.1, which consists of a high resistivity oxide layer (top layer) fixed on a metal-rich less resistive layer (base layer) sandwiched between two metal electrodes. The TaO_x layer is highly doped with oxygen vacancies (V_O) which behave like n-type semiconductor and its resistance is assumed to be R_B . This resistance is assumed to be constant during the whole switching cycles. D is the thickness of the Ta₂O₅ layer and its resistance R_I . The resistance of the Ta₂O₅ oxide layer is variable due to the drifting of oxygen vacancies in and out of the layer during the RS mechanism. The thickness of these layers varies from 2-5 nm and 10-50 nm for the top and base layers, respectively [17]. In this chapter, the thickness of the insulating layer Ta₂O₅ is 4-nm which can be changed to fit the different available bi-layered RRAM models of the same structure. The term w is used to refer to the length of the un-doped region in the CF. The doped region is the CF region with high concentration of donor-like oxygen vacancies (the low resistance region of the CF). Similar to the previous work [1], [16] the Pt BE will be grounded and all the applied voltages and simulation measurements will take place on the TE which is an independent metal layer that is unaffected by the switching mechanism [30].

4.1.2. The Bipolar Resistive Switching Mechanism of the Proposed Model

Low Resistance State: LRS is reached when a negative voltage is applied as in Figure 4.1(a).

In this case, oxygen ions in the Ta₂O₅ layer and in the vicinity of the interface region will be

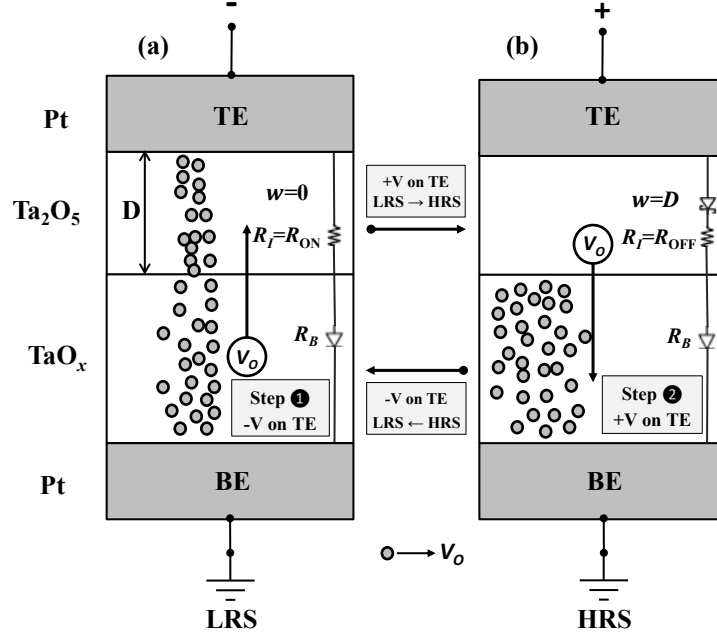


Figure 4.1. A schematic representation of the proposed mathematical RRAM model and its BRS mechanism. (a) The LRS and (b) the HRS [21].

pushed toward TaO_x layer, leaving behind donor-like oxygen vacancies which dope the Ta₂O₅ layer [1]. This results in a metal rich doped region and reduces the barrier height ϕ_b , simultaneously. ϕ_b is the potential barrier height for electrons moving from TE→TaO_x (Schottky-like barrier). When all the length of Ta₂O₅ layer is doped ($w=0$), the RRAM reaches its LRS and the Schottky-like interface between TE and Ta₂O₅ is changed into ohmic interface. This is shown in Figure 4.1(a) by step 1 where the arrow inside the cell signifies V_o movement direction. However, for tantalum oxide, the defect states due to V_o act as electron donors [55]. Thus, the drifting of V_o into the doped region increases the electron concentrations and hence, Fermi level increases [17]. Accordingly, a reduction of Schottky barrier height ϕ_b transpires [17] and a forward current is resulted in the direction TE→TaO_x. A contrasting effect happens while switching into HRS.

High Resistance State: When a positive voltage is exerted [Figure 4.1(b)], oxygen ions migrate from the bulk layer toward Ta₂O₅ layer and the interface region (the oxygen vacancies are repelled away from Ta₂O₅ layer) which un-dope the Ta₂O₅ layer and increases the barrier height (the ohmic interface is changed back to Schottky-like interface). Consequently, the RRAM state is changed into HRS when all the length of the Ta₂O₅ layer is un-doped ($w=1$). This state change is indicated in Figure 4.1(b) by step 2.

4.2. Modelling Of The un-Doped Region Evolution Stages

4.2.1. Modelling of Oxygen Ion Migration for Ta₂O₅/TaO_x RRAM

The doped region evolution for the Ta₂O₅/TaO_x RRAM is believed to be based on the ionic drift mechanism [1] which can be explained using Mott and Gurney rigid point-ion model [56], [57]. According to Mott, oxygen ions hop in the net potential of constituent ions where the migration of an ion between two sites requires a certain amount of energy in order to overcome a potential barrier. The degree of barrier lowering and the oxygen ions migration rate are proportional to the electric field in the ions hopping active region (un-doped region) E [18], [58]. However, under no bias, the chance per unit time that an oxygen ion can hop over the barrier into an oxygen vacancy position is given by [56]:

$$c \cdot \exp\left(-\frac{U}{kT}\right) \quad (1)$$

where c is the attempt-to-escape frequency, U is the intrinsic barrier for ion hopping, and kT is the thermal energy. When a field is applied, U is lowered by $\frac{1}{2}qaE$ for oxygen ions moving

in the opposite direction of the field [56]. Thus, oxygen ions movement probability in that direction increases to:

$$c \cdot \exp\left\{-\frac{\left(U - \frac{1}{2}qaE\right)}{KT}\right\} \quad (2)$$

where a is the effective hopping distance and q is the electron charge. Simultaneously, ions hopping probability in the opposite direction decreases by the same amount. For the proposed model to be in consistent with Mott-Gurney model, the ionic drift equation derived in this work is assumed to be for oxygen ions (instead of vacancies). The growth rate of w is then given by the average ionic drift velocity of oxygen ions $v(t)$:

$$\frac{dw}{dt} = v(t) = v_{-E} - v_E \quad (3)$$

$$\begin{aligned} &= a \cdot c \cdot \exp\left(-\frac{U}{KT}\right) \left\{ \exp\left(\frac{\frac{1}{2}qaE}{KT}\right) - \exp\left(-\frac{\frac{1}{2}qaE}{KT}\right) \right\} \\ &\approx a \cdot c \cdot \exp\left(-\frac{U}{KT}\right) \cdot \sinh \frac{E}{E_0} \end{aligned} \quad (4)$$

where $E_0 = \frac{2KT}{qa}$, v_E and v_{-E} are ionic drift velocity along and opposite to the direction of the field, respectively. The complete evolution of w along the RS cycle is assumed to be proportional to $v(t)$. Thus, (4) is assumed to describe the kinetics of the SET/RESET processes in the RS. Also, different from Ta/TaO_x structure [59], any lateral evolution of oxygen ions is assumed to be ignored. However, for $v(t)$ to be used in the simulation, the dynamics of w are initially modelled.

4.2.2. Modelling of the Un-Doped Region Dynamics During the Simulation

The change in w is calculated by assuming that $v(t)$ represents the growth rate over the time span $[b_1, b_2]$ where b_1 is the bias starting time and $b_2 = N/f$. N is the number of the bias cycles and f is the frequency. By dividing $[b_1, b_2]$ into P time intervals $[t_0, t_1, \dots, t_P]$ of equal length Δt (5), where $[b_1=0=t_0 < t_1 < t_2, \dots, t_P=b_2]$, then $v(t_{i-1})$ represents the growth rate at the beginning of the i_{th} interval where $i = 1, 2, \dots, P$.

$$\Delta t = \frac{b_2 - b_1}{P} = \frac{N}{fP}. \quad (5)$$

For small Δt , good approximation of the change in w over i_{th} time interval is obtained as follows:

$$v(t_{i-1}) \cdot \Delta t. \quad (6)$$

Therefore, the approximate total changes in w over the time period $i=1-i=P$ is given by:

$$\begin{aligned} w &\approx \sum_{i=1}^P v(t_{i-1}) \cdot \Delta t \\ &= \sum_{i=1}^P a \cdot c \cdot \exp\left(-\frac{U}{kT}\right) \cdot \sinh \frac{E_i}{E_0} \cdot \Delta t. \end{aligned} \quad (7)$$

If $E_i < E_0$, the \sinh term is reduced to $\frac{E_i}{E_0}$ and $v(t_{i-1})$ drops significantly. Thus, w stops changing. Similarly, at $E_i > E_0$, the \sinh term is reduced to $-\exp \frac{E_i}{E_0}$ and $\exp \frac{E_i}{E_0}$ for the switching stages (HRS→LRS) and (LRS→HRS), respectively and hence, E_i contributes significantly to $v(t_{i-1})$ and w value starts shifting. This dynamic is in agreement with the physics of thin film RRAM where the ionic drift velocity is not proportional to the applied field; instead, it has a nonlinear relationship with the field [57]. The acquisition of E_i in (7) is explained in the next section.

4.2.3. Electric Field Modelling for the Proposed Model

The electric field E is estimated by using the voltage drop on the un-doped region V_U as follows:

$$E = \frac{V_U}{w}. \quad (8)$$

Assuming the voltage across Ta_2O_5 layer V_D comprises two variable voltages across the doped and un-doped parts and using a voltage division [9], V_U can be estimated as follows:

$$\begin{aligned} V_U &= V_D \frac{R_U}{R_U + R_D} \\ &= V_D \frac{R_{\text{OFF}} \cdot w / D}{R_{\text{OFF}} \cdot w / D + R_{\text{ON}} \cdot (D - w) / D} \end{aligned} \quad (9)$$

where R_U and R_D are assumed to be the variable resistances of the un-doped and doped regions of the insulator layer, respectively. In (9), the resistance of Ta_2O_5 layer is assumed to be R_{ON} and R_{OFF} for the LRS and HRS, respectively (see Figure 4.1). Also, it is assumed that R_U and R_D change in accordance to the change in w (because the change in w is proportional to the change in the density of oxygen ions in the Ta_2O_5 layer which in turn reflects the change in the resistance). Substituting (9) into (8) yields:

$$E = \frac{V_D}{w + R_r(D - w)} \quad (10)$$

where $R_r = \frac{R_{\text{ON}}}{R_{\text{OFF}}}$.

To find V_D , all voltage drops across the cell are considered. An intrinsic Schottky barrier exists between TE and Ta_2O_5 layers while in HRS and its height is reduced until the contact is changed into ohmic at LRS [1]. The contact voltage is assumed to be V_S . Thus, the contact and the Ta_2O_5 layer can then be modelled as a variable Schottky diode (represent a variable Schottky barrier) connected in series with a variable resistor $R_t = R_U + R_D$, as in Figure 4.1. Finally, since the

RS is based on the rupture/formation of the doped region within the Ta₂O₅ layer then, the bulk layer is assumed to behave as a series constant resistor R_B and its voltage is IR_B (see Figure 4.1). Thus, V_D is given by:

$$V_D = V - IR_B - V_S. \quad (11)$$

$$= \left(R_{\text{ON}} \left(1 - \frac{w}{D} \right) + R_{\text{OFF}} \cdot \frac{w}{D} \right) \cdot I = R_I \cdot I. \quad (12)$$

The contact voltage V_S is given by:

$$V_S = V - I(R_{\text{series}}) \quad (13)$$

where $R_{\text{series}} = R_I + R_B$ is the total resistance in series with Schottky contact. In (10), the nanoscale nature of w reflects the high electric field which contributes to the intrinsic nonlinearity of $v(t)$. Other intrinsic features of the threshold and the self-limiting effect are explained for both, switching into LRS and HRS in the next two sections.

4.2.4. The Electric Field Threshold and the Self-limiting Effect During Switching Into LRS

During the switching stage (HRS→LRS), E increases with V_D , following (10). Eventually, the sinh term in (7) is reduced to $-\exp \frac{E_i}{E_0}$ when $E_i > E_0$ and w starts decreasing after that as follows:

$$w = \sum_{i=1}^P -a \cdot c \cdot \exp\left(-\frac{U}{KT}\right) \cdot \exp \frac{x_1 |E_i|}{E_0} \cdot \Delta t. \quad (14)$$

where x_1 is the enhancement fitting factor of the electric field E_i dependence.

At certain value of the field ($E_{\text{HRS} \rightarrow \text{LRS}}$) in the region $E_i > E_0$, $v(t)$ will be high enough (has a

significant contribution on the nanoscale term w) to trigger the abrupt switching property and w reaches 0, abruptly. The required voltage to reach this value is called LRS switching voltage (LSV) as can be seen in Figure 4.2. Simultaneously, the depleted gap at the un-doped region is refilled by oxygen vacancies when LRS is reached ($w = 0$). Thus, E is no longer applied on the active region [18]. This effect leads to the self-limiting of set transition by suppression of oxygen ions migration and hence, limiting the generation of its corresponding oxygen vacancies. At $w = 0$, E reaches its LRS value E_{LRS} as in (15) which can be further increase if the bias kept increasing after the switching.

$$E_{\text{LRS}} = \frac{V_D}{R_T D}. \quad (15)$$

This reveals the high $v(t)$ that the device reaches at LRS, which if used directly in our model, w will drop below 0 when the cell remains under bias. However, since the permissible physical values of w is limited to $[0, D]$, (7) is modified by forcing $v(t_{i-1})$ value to be identical to zero once the cell reaches its LRS physical limit ($w = 0$) as follows:

$$v(t_{i-1}) \approx 0 \text{ when } w \leq 0. \quad (16)$$

The field that is experienced by ions migration is the local electric field. However, since it is difficult to estimate the exact value of the local field strength, the proposed model used the average field where x_1 in (14) accounts for the ion hopping dependency on the electric field.

4.2.5. The Electric Field Threshold and the Self-limiting Effect During Switching Into HRS

Similar to the switching into LRS, during the switching stage (LRS→HRS) and when $E > E_0$, w starts increasing, following (14) but with the negative sign is neglected and the enhancement fitting factor is changed to x_2 . Following the same explanation in the previous stage, the voltage required to trigger the switching is called the HSV (see Figure 4.2). This is the voltage required for the field to reach a high enough value ($E_{\text{HRS} \rightarrow \text{LRS}}$) that drive $v(t)$ to have significant influence on the nanoscale term w . Eventually, E decreases to its HRS value E_{HRS} when $w = D$ as follows:

$$E_{\text{HRS}} = \frac{V_D}{D}. \quad (17)$$

Although E_{HRS} is smaller than E_{LRS} and $v(t)$ drops significantly compared to its value when $w=0$, $v(t)$ still can forces w to keep increasing but at a smaller growth rate. Thus, (7) is further modified to reflect the permissible physical value of w $[0, D]$ as follows:

$$v(t_{i-1}) \approx 0 \quad \text{when } w \geq D. \quad (18)$$

Therefore, for all the values of V , the growth rate of the un-doped region is given by:

$$v(t_{i-1}) \approx \begin{cases} v_{1,2} \cdot a \cdot c \cdot \exp\left(-\frac{U}{KT}\right) \cdot \sinh \frac{x_{1,2} E_i}{E_0}, & 0 < w < D \\ 0, & 0 \geq w \geq D \end{cases} \quad (19)$$

where v_1 and v_2 are fitting parameters account for the vertical growth/dissolution velocity. By substituting (10) and (19) in (7), we get w .

4.3. Current–Voltage Behaviour

4.3.1. Current Transport Process in the Proposed Mathematical Model

Since the proposed model is based on Schottky barrier modulation and tunnelling, the dominant conduction current is due to the majority carriers (electrons) [1], [16], [32]. However, at thermal equilibrium, unbiased condition, and when the effects of the insulator layer and image force lowering [32] are ignored, the flow of electrons in the direction $\text{TaO}_x \rightarrow \text{TE}$ and the opposite flow $\text{TE} \rightarrow \text{TaO}_x$ are equal, resulting in a total zero current. Both of these current components are proportional to the carrier's density at the boundary and it can be approximated as follows [32], [60]:

$$|I_{\text{TE} \rightarrow \text{TaO}_x}| = |I_{\text{TaO}_x \rightarrow \text{TE}}| = AA^*T^2 \exp\left(-\frac{\phi_{\text{Bn0}}}{V_T}\right) \quad (20)$$

where $I_{\text{TE} \rightarrow \text{TaO}_x}$ and $I_{\text{TaO}_x \rightarrow \text{TE}}$ are the current components in the directions $\text{TE} \rightarrow \text{TaO}_x$ and $\text{TaO}_x \rightarrow \text{TE}$, respectively. A is the electrode area, A^* is Richardson constant, and T is the temperature. ϕ_{Bn0} is the ideal Schottky barrier height when an n-type semiconductor is used. V_T is the thermal voltage which equals to $(kT/q \approx 26 \text{ mV})$ where k is the Boltzmann constant. When a forward bias V is applied, the barrier height decreases and hence, the surface charge carrier density is increased. This allows the electrons to move easily in the direction $\text{TE} \rightarrow \text{TaO}_x$. The potential difference across the barrier is reduced by an amount equal to the voltage drop across Schottky barrier V_S . For forward bias, the total net current I_F can be expressed as follows [32], [61], [60]:

$$I_F = AA^*T^2 \exp\left[-\frac{(\phi_{\text{Bn0}} - V_S)}{V_T}\right] - AA^*T^2 \exp\left(-\frac{\phi_{\text{Bn0}}}{V_T}\right) \quad (21)$$

$$= AA^*T^2 \exp^{-\phi_{\text{Bn0}}/V_T} [\exp^{\frac{V_S}{V_T}} - 1] \quad (22)$$

where V_S is given in (13). The first and second terms in (21) are the current components in the direction $TE \rightarrow TaO_x$ and the opposite direction, respectively. The reverse current can be obtained using the same expression in (22) but with reversing the polarity of V_S and the direction of the current [60].

4.3.2. Adding the Effect of the Insulator Layer–TPF

In thin insulators, and under high electric field, the tunnelling process can be the common carrier conduction mechanism [32], [60]. This is a result of quantum mechanics where the electron wave function can penetrate through the potential barrier. The insulator between the metal and semiconductor layers reduces the majority-carriers current and also results in a higher ideality factor [32] which leads to the deviation from the ideal thermionic emission mechanism. The proposed mathematical model emphasizes these two deviation effects by considering the quantum tunnelling in the insulator layer [32], [61], [62]. This tunnelling mechanism relies on the thickness of the insulator layer as follows.

Very Thin Insulator Layer (<1nm): The carriers do not encounter resistance in the transporting process and the conduction follows the ideal Schottky contact equation (22).

An Insulator Layer Thickness (>1nm): Tunnelling starts when Ta_2O_5 thickness is > 1 nm and the conduction can be assumed to follow the tunnelling process in the MIS system. This approximation is valid for MISM devices with high electric field and an insulator layer of a specific thickness only.

Thick Insulator Layer: The tunnelling current is reduced by increasing the insulator layer thickness [32]. At a thick enough insulator layer, most of the electron tunnelling transportation through the interface is negligible. As a result, the tunnelling approximation cannot be used for all the available bi-layered RRAM physical models where the insulator layer in some models is thick enough that the tunnelling effect is ignored and other mechanism dominate the conduction. It has been theorized in [32] that the tunnelling can occur in an insulator layer of few nanometre thickness only. According to [17], the usual thickness of the insulator layer in the Ta₂O₅/TaO_x RRAM is 2–5 nm which is in the reasonable range for the tunnelling to occur [32]. However, the proposed model successfully reproduced the behaviour of Ta₂O₅/TaO_x RRAM physical model with an insulator layer of 4 nm (and 3 nm as in Chapter Five).

Although increasing the insulator layer thickness reduces the tunnelling effect, it is important to include it in the conduction equation when the insulator layer thickness is still under the threshold value. The reduced current is resulted from the added interfacial layer Ta₂O₅. The explained tunnelling effect can be achieved by adding the term TPF $\left(\exp^{-\sqrt{\xi}w \times 10^{10}}\right)$ [32] as can be seen in (23). TPF depends on the insulator layer physical characteristics and it determines the probability of the tunnelling current through the RRAM barrier. The added term reduces the device current significantly and hence, reflecting the first effect of the insulator layer mentioned in the previous chapter. The tunnelling current is thus given by:

$$I_F = AA^*T^2 \exp^{-\frac{\phi_{Bn0}}{V_T}} \left(\exp^{\frac{(V-IR_{series})}{V_T}} - 1 \right) \left(\exp^{-\sqrt{\xi}w \times 10^{10}} \right) \quad (23)$$

where ξ is the effective barrier height which is used as a fitting parameter and $w \times 10^{10}$ is the thickness of the insulator volume in Å. This is the total current through the device which consists of both tunnelling and thermionic emission [32], [61]. The expression for the reverse bias condition is similar to (23) except that the polarity of Schottky potential and the current direction are reversed.

Another factor which reflects the deviation from the ideal equation, called the ideality factor η , is added to the memristor characteristic equation (23) as follows:

$$I_F = AA^*T^2 \exp^{-\frac{\phi_{Bn0}}{V_T}} \left(\exp^{\frac{(V-IR_{series})}{\eta V_T}} - 1 \right) \left(\exp^{-\sqrt{\xi} w \times 10^{10}} \right). \quad (24)$$

The term η is a unit-less parameter which is a measure of the deviation of the system from the pure thermionic emission mechanism of Schottky barrier. This deviation arises due to the existence of the insulator layer and interface traps [32], [61], [63].

With no tunnelling, η and TPF are equal to unity and the current is determined by the thermionic emission equation [32], [61]. Conversely, at high field, and when the insulator thickness exceeds 1 nm, tunnelling starts, and the value of η exceeds 1, which indicates that the thermionic emission current is no longer the dominant conduction in the system and other mechanism is dominating the current conduction (e.g. tunnelling barrier) [32]. Simultaneously, the value of TPF starts to decrease; reducing the current through the device (indicates tunnelling).

The interface traps available at the interface of the semiconductor play an important role in determining the conduction current in the bi-layered RRAM device. Hence, an accurate RRAM model with robustness should include the effect of these traps.

4.3.3. The Effect of the Continuous Charging–Discharging of the Interface Traps on the I – V Behaviour

Forming of the Interface Traps: The interface traps in the MIS devices are a property of the semiconductor layer [62]. However, before going through the modelling of the interface traps effect in the bi-layered RRAM, it is important to understand how these traps are originally being formed in the MIS device. The atoms at the surface of the semiconductor layer have neighbours on one side only and their valence electrons at the vacuum side have no partners which can be used to form covalent bonds. Instead, these atoms have one unpaired electron situated in a localized orbital (dangling bond) directed away from the surface [62]. The interface traps are the electronic states which have been formed by these dangling bonds. The dangling bonds act as traps and can behave as donors or acceptor by giving up or accepting an electron, respectively. If the interface traps are occupied up to a certain energy level called the neutral level (the electrically neutral trapping potential well which can bind only 1 electron or a hole [61], [64]) and all the states above it are empty, then the semiconductor surface is electrically neutral. This is considered as a very rare case that seldom occurs in the experimental results. Thus, usually there are some charges in the interface traps of the RRAM as described next [62].

The Effect of the Thickness of the Insulator Layer on the Interface Traps Density: As in the MIS system, for the MISM RRAM studied in this research, the interface traps can be divided into two groups. The first group can communicate readily with the semiconductor while the other one communicates with the metal. Hereafter, these groups will be referred to as type

1 and 2, respectively. The densities of the groups are function of the insulator layer thickness (δ). According to this classification, the Ideality factor is given as follows [32], [61]:

$$\eta = 1 + \frac{(\delta/\varepsilon_o)(\varepsilon_s/W + qD_1)}{1 + (\delta/\varepsilon_o)qD_2} \quad (25)$$

where ε_o is the dielectric constant of the insulator, ε_s is the dielectric constant of the bulk layer, W is the depletion layer thickness, and D_1 and D_2 are the interface traps densities of type 1 and 2, respectively. However, the thickness of the insulator layer can alter the interface traps density and leads to the deviation from the ideal Schottky barrier conduction equation. By knowing that all the traps are located at the insulator-semiconductor interface, the communication between D_2 and the metal increases for smaller insulator layer while that of D_1 increases for thicker δ . If δ is thick enough (≥ 3 nm), then the value of η is largely determined by D_1 and thus, $D_2 \approx 0$ [32], [61] Equation (25) is reduced to:

$$\eta_{D_2=0} = 1 + (\delta/\varepsilon_o)(\varepsilon_s/W + qD_1). \quad (26)$$

The term $\delta\varepsilon_s/W\varepsilon_o$ can be neglected [61] which would eventually yield a rigorous interpretation of the interface traps density term $\eta_{D_2=0}$ as follows:

$$\eta_{D_2=0} = 1 + (\delta/\varepsilon_o)(qD_1). \quad (27)$$

Since the main contribution to the variation in $\eta_{D_2=0}$ is attributed to the change in D_1 , either (26) or (27) can be used which would eventually lead to the similar approximation. In this case, D_1 tends to increase the value of $\eta_{D_2=0}$ [32]. Similarly, if δ is below 3 nm, most of the interface traps become in equilibrium with the metal which means that $D_1 \approx 0$. Equation (25) becomes:

$$\eta_{D_1 \rightarrow 0} = 1 + \frac{(\delta/\varepsilon_o)(\varepsilon_s/W)}{1 + (\delta/\varepsilon_o)qD_2}. \quad (28)$$

In this case, D_2 does not have a momentous impact on the value of η . This can clearly reflect the fact that when δ is very small, the value of η approaches unity, which represents an ideal Schottky barrier conduction mechanism. However, since δ in the proposed RRAM model is assumed to be 4 nm (the experimental data in [16] is based on 4 nm insulator layer), η is assumed to follow $\eta_{D_2=0}$.

The Continuous Charging–Discharging of the Interface Traps: The most crucial feature of the interface traps equation given in (26) is the continuous changing values of D_1 and $\eta_{D_2=0}$ along the RS cycles. When a bias is applied for RS, Fermi level moves continuously up or down with respect to the interface traps levels where the degree of bending is proportional to the applied bias [32]. This movement results in a continuous change of the charge of the interface traps [61] which in turn affects the magnitude of the interface traps density on the semiconductor, continuously.

During RS, the surface charge carrier density is continuously increased or decreased. However, since the density of the interface traps D_1 increases by increasing the number of mobile charge carriers moving into the interface [61], [65] which is the case of a forward bias, thereupon, the values of D_1 and hence, $\eta_{D_2=0}$, continuously increase and decrease as the state is switched to LRS and HRS, respectively. The values of D_1 and $\eta_{D_2=0}$ will reach their maximum value at LRS ($w = 0$) and will start decreasing again toward smaller values once a reverse bias is applied. These two parameters will reach their minimum values when $w = 1$ at HRS. This continuous changing mechanism can be modelled as a function of the state variable as follows:

$$\eta = \left(\eta_{D_2=0, D_1(\text{LRS})} \right) \left(1 - \frac{w}{D} \right) + \left(\eta_{D_2=0, D_1(\text{HRS})} \right) \frac{w}{D} \quad (29)$$

where:

$$\eta_{D_2=0, D_1(\text{LRS})} = 1 + (\delta/\varepsilon_o)(qD_1(\text{LRS})) \quad (30\text{-a})$$

and

$$\eta_{D_2=0, D_1(\text{HRS})} = 1 + (\delta/\varepsilon_o)(qD_1(\text{HRS})) \quad (30\text{-b})$$

where $D_1(\text{LRS})$ and $D_1(\text{HRS})$ are the interface traps densities at LRS and HRS, respectively. Nevertheless, there is uncertainty about the value of ε_o which depends on δ [61]. Therefore, a model using the whole equation of η is difficult to be achieved. The values of η at the two limiting cases of LRS (η_{LRS}) and HRS (η_{HRS}) can be estimated by fitting η into (24) to get the best I - V fitting when compared to the measured data in [16] or in other physical model. These values can then be used in (29) to get the best I - V behaviour for the proposed RRAM when compared to the experimental results. To get the best fitting results, a fitting parameter m is added to (29) as follows:

$$\eta = m[(\eta_{\text{LRS}})(1 - \frac{w}{D}) + (\eta_{\text{HRS}})\frac{w}{D}] \quad (31)$$

In this section, it has been shown the impact of the continuous changing of the interface traps densities located at the semiconductor interface on the bi-layered RRAM current conduction process during RS cycles. This was achieved by employing the physics of the semiconductor of the RRAM layers and by relating the thickness of the active oxide layer in the RRAM to the interface traps densities. The values of the trapped charges are changing as long as the applied voltage is varying. However, only two discrete values of the interface charges densities and η

do not reflect the actual situation. It is incorrect to assume only two discrete values for these two parameters at the forward and reverse bias operation.

4.3.4. Adding the Effect of the Image Force Lowering Factor and the Doping Level Variation on Schottky Barrier

The barrier height ϕ_{Bn0} is lowered owing to image force lowering [32] and the presence of the electric field. The image force lowering factor $\Delta\phi$ is small compared to the barrier height itself ($q\phi_{Bn0} \approx 0.6 \text{ eV}$) and it does not have large impact on the I – V behaviour. The value of $\Delta\phi$ is given by [32]:

$$\Delta\phi = \left[\frac{q^3 N \varphi_s}{8\pi^2 \epsilon_s^3} \right]^{1/4} \quad (32)$$

where N is the bulk layer charge density. The value of φ_s is given by the following equation [32], [61]:

$$\varphi_s = \phi_{Bn} - \phi_n \pm V_s \quad (33)$$

where ϕ_{Bn} is the variable Schottky barrier and ϕ_n term has a significantly small value that can be ignored.

Another factor which influences Schottky barrier in the bi-layered RRAM is the lengths of the doped and un-doped regions. The resistance of the switching layer decreases/increases by increasing/decreasing the number of oxygen vacancies in it. As a result, Schottky barrier will have a variable height and reaches its maximum value at HRS when the number of oxygen vacancies in the Ta_2O_5 layer reaches its minimum value. After that, it decreases again during switching to LRS until it disappears when Ta_2O_5 layer is fully doped (ohmic contact). Since

the doped and un-doped regions of the Ta₂O₅ layer are corresponding to w variation when it is approaching 0 and 1 respectively, their effect can be modelled as in the following equations:

$$\phi_{Bn} = \phi_{Bn0} \frac{w}{D}. \quad (34)$$

Therefore, Schottky barrier height is reduced by two different factors simultaneously. The main reduction is determined by the doped and un-doped regions whereby the other factor of image force lowering involves a significantly smaller effect. These two parameters are combined in the following equation:

$$\phi_b = \phi_{Bn} - \Delta\phi. \quad (35)$$

$$\phi_b = \phi_{Bn0} \left(\frac{w}{D} \right) - \left[\frac{q^3 N \phi_s}{8\pi^2 \epsilon_s^3} \right]^{1/4}. \quad (36)$$

In (33), since ϕ_n is significantly smaller than the other two parameters in the equation [7], it can be ignored. In addition to that, (33) was stated in [32] and [60] to represent the potential barrier for an MIS system in which Schottky barrier height depends on the applied voltage. However, in the proposed model, since Schottky barrier value is changing according to the doped and un-doped regions which in turn depends on the voltage, then the effect of the applied voltage is already being incorporated and can be ignored in (33). Thus:

$$\phi_s \approx \phi_{Bn}. \quad (37)$$

After introducing Schottky barrier lowering effects and the ideality factor into (24), the Ta₂O₅/TaO_x RRAM I - V equation becomes:

$$I = AA^* T^2 \exp^{-(n_{1,2} \phi_b)/V_T} \left(\exp^{\frac{(V - IR_{series})}{\eta V_T}} - 1 \right) \left(\exp^{-\sqrt{\xi} w \times 10^{10}} \right). \quad (38)$$

Equation (38) represent the electronic current not the ionic current (which only has a very specific transient current during the switching event). However, for the simplification of the model, we assumed that T_0 is the device temperature when it is not in the switching stage (at LRS or HRS) and hence, T_0 is used in (38). n_1 and n_2 are fitting parameters that determine the influence of ϕ_b on I .

4.4. Temperature Modelling

During RS process, the formation and rupture of the CF are sensitive to the temperature. Thus, the temperature effect is important during the RS behaviour and should be considered in the CF growth rate equation. The temperature in the simulation is the local temperature around the doped region which can be raised during the RS due to Joule heating effect [66]. This enhances the ions migration process and thus, it should be used in the growth rate equation. For the simplification of the model and since the current work focuses on other physics aspects, the approximate value of the temperature used in this model is based on the simple analysis in [58] and [66]. A complete electro-thermal analysis has already presented in the literature and can be used in the future work. The doped region temperature is given by [66]:

$$T = T_0 + I^2 \cdot R \cdot R_{th} \quad (39)$$

where T_0 is the ambient temperature, R_{th} is the effective thermal resistance, R is the doped region electrical resistance, and I is the current through that region.

4.5. Bi-Layered RRAM Device Simulation and Results Discussion

The RRAM equations provided in sections 4.2–4.4 have been evaluated by simulation using MATLAB. The full MATLAB code is provided in Appendix A. The device coefficients used during the simulation includes the following: $R_{ON} = 1.7 \text{ k}\Omega$, $R_B = 12 \text{ k}\Omega$, $R_{OFF} = 40 \text{ k}\Omega$ s, $D = 4 \text{ nm}$, $A = 9 \times 10^{-6} \text{ cm}^2$, $A^* = 120 \times 10^4 \text{ A} \cdot \text{m}^{-2} \cdot \text{K}^{-2}$, $\phi_{Bn0} = 0.6 \text{ eV}$, $c = 1 \times 10^{13} \text{ Hz}$, $U = 1 \text{ eV}$, $x_1 = 175$, $x_2 = 0.4$, $T_0 = 300 \text{ K}$, and $a = 1 \text{ nm}$ [67] which can be used as fitting parameter to account for the un-doped region growth velocity. The initial conditions presumed that the RRAM state is at LRS with an initial resistance $R_{series} = R_{ON} + R_B$ and $w = 0 \text{ nm}$. The proposed model is correlated against several published characteristics of the Pt/Ta₂O₅/TaO_x/Pt RRAM and a number of different insights and matched features emerged.

4.5.1. Relationship and the Agreement with the LRS/HRS Switching Behaviour

4.5.1.1. Non-Linear Ionic Drift Mechanism

Figure 4.2 shows the measured data for the fabricated Pt/Ta₂O₅/TaO_x/Pt [16] compared with the simulated semi-log scale plot of the I – V characteristic of the BRS mathematical proposed model for both SET and RESET processes. It can be seen that the device is switching to LRS and HRS periodically by a 100 Hz sine wave, SET voltage of -2 V and 3 V RESET voltages

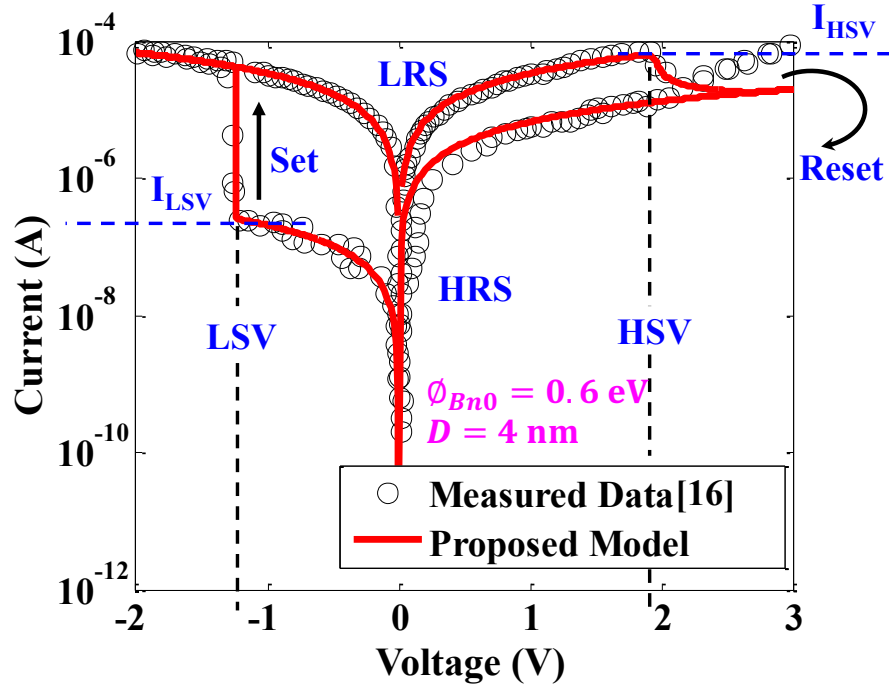


Figure 4.2. Experimental measurements [16] and the semi-log scale plot of the modelling results I - V characteristics with $D = 4$ nm [21].

and the simulation result exhibits a good agreement with the results of the experimental measurement for the same RRAM structure cell. Also, it is shown that the resistance decreases under a negative voltage and increases when the reverse polarity is applied. In addition, the rectifying behaviour in the HRS was clearly observed which indicates the formation of the variable Schottky barrier.

However, this barrier and the variable resistance layer (Ta_2O_5) lead to the asymmetry phenomena in the RRAM characteristics while it is in the HRS [1]. Figure 4.2 shows a symmetric current profile while the device is in the LRS and asymmetric behaviour while it is in the HRS. This is another attributes that matches with the experimental results and proves the accuracy of the proposed model. Likewise, the model can reproduce the abrupt switching property in the resistance value at around $\text{LSV} \approx -1.2$ V and a less abrupt switching at $\text{HSV} \approx$

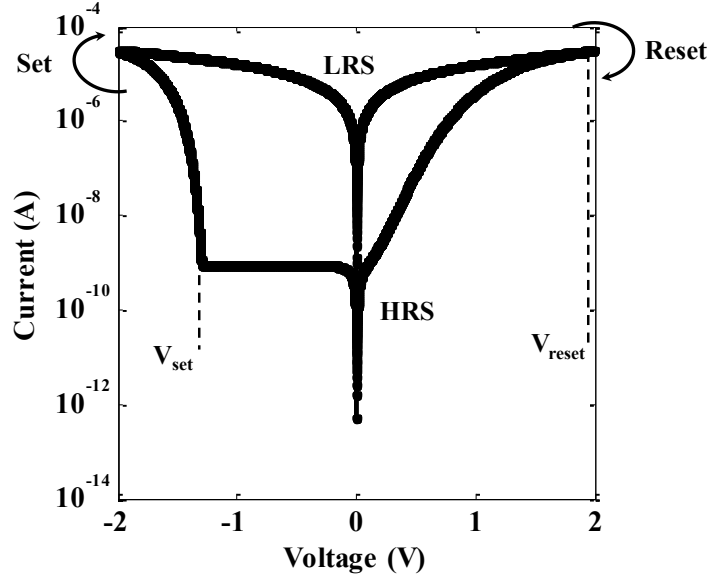


Figure 4.3. Semi-log scale plot of the I - V characteristics of the proposed RRAM mathematical model with the addition of TPF and the continuous variation of the interface traps densities but with using linear dopant drift model

1.9 V for SET and RESET processes, respectively. Furthermore, the proposed model predicted the transition from linear to non-linear behaviour for the LRS and HRS, respectively.

Figure 4.2 is used to discuss the small deviation observed in the RESET switching which has not been explored or discussed in the previous bi-layered RRAM models. In the physical $\text{Ta}_2\text{O}_5/\text{TaO}_x$ RRAM device, when RESET occurs at HSV = 1.9 V (see measured data in Figure 4.2), the CF switches to its HRS and most of the applied voltage is applied on the Ta_2O_5 layer due to its higher resistance compared to R_B . However, due to the large area of the Ta_2O_5 region outside the CF (OCF) compared to the CF itself, this area can act as a highly nonlinear insulator switch in parallel with the CF [8]. When the applied voltage increased further (after RESET), the conductance of OCF considerably increased [8]. Hence, the total resistance of the Ta_2O_5 layer decreased which is reflected in the experimental results in Figure 4.2. However, for simplicity, OCF is considered inactive in the proposed model (the total HRS is fixed) and all

the other $\text{Ta}_2\text{O}_5/\text{TaO}_x$ RRAM models which is the reason of the observed deviation in Figure 4.2 and resulted in a maximum error of 70%. However, the average error is $< 11\%$ which can be further reduced in the future by taking OCF into account. The same deviation is observed in Figure 4.8, Figure 5.4, Figure 5.5, and Figure 5.6.

4.5.1.2. Ideal State – Linear Dopant Drift

Figure 4.3 shows the simulated semi-log scale plot of the I - V characteristic of the BRS proposed model, using the simple ideal ionic drift equations given by [9]. Similar to the case of the non-linear ionic drift mechanism, it can be seen in that the device is switching ON and OFF periodically by a 100 Hz sine wave $V = 2 \sin(\omega_0 t)$ but does not exhibits a good agreement with the results of the experimental measurement for the same RRAM cell structure fabricated in previous publications [16], especially at the switching regions. However, the device shows the correct LRS and HRS current levels. These results show the importance of using the correct physics involved during the RS process of the bi-layered RRAM (non-linear

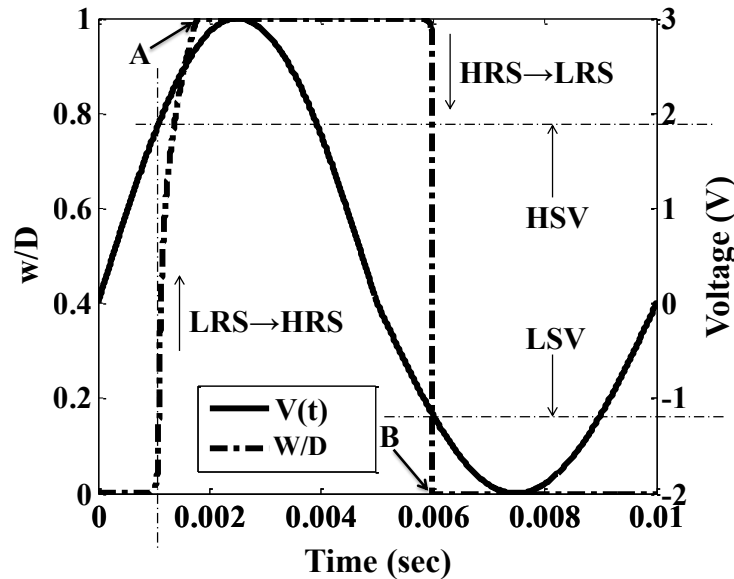


Figure 4.4. Calculated w normalized to D and the total applied bias as a functions of time [21].

ions hopping mechanism).

4.5.2. The Complete Evolution of w , ϕ_b - V , and R_{series} - V

The time dependence of w normalized to D is plotted together with V against time in Figure 4.4 while Figure 4.5 presents the evolution of ϕ_b - V and R_{series} - V curves during the RS. It can be seen in Figure 4.4 that w varies between 0 and 1, corresponding to 0–4 nm, for the switching into LRS and HRS, respectively. Figures Figure 4.4 and Figure 4.5 compare the change in w and the corresponding variation in ϕ_b [Figure 4.5(a)] and R_{series} [Figure 4.5(b)]. The results show that during the switching (HRS→LRS) and before reaching LSV, the parameters w , ϕ_b , and R_{series} are fixed at their maximum value ($\phi_b = \phi_{\text{Bn}} - \Delta\phi \approx 0.58$ eV). The values of ϕ_b (36) and R_{series} (13) depend on the evolution of w which in turn start decreasing abruptly once LSV is reached, to eventually reach 0 (Figure 4.4) and hence, force ϕ_b and R_{series} to drop to 0

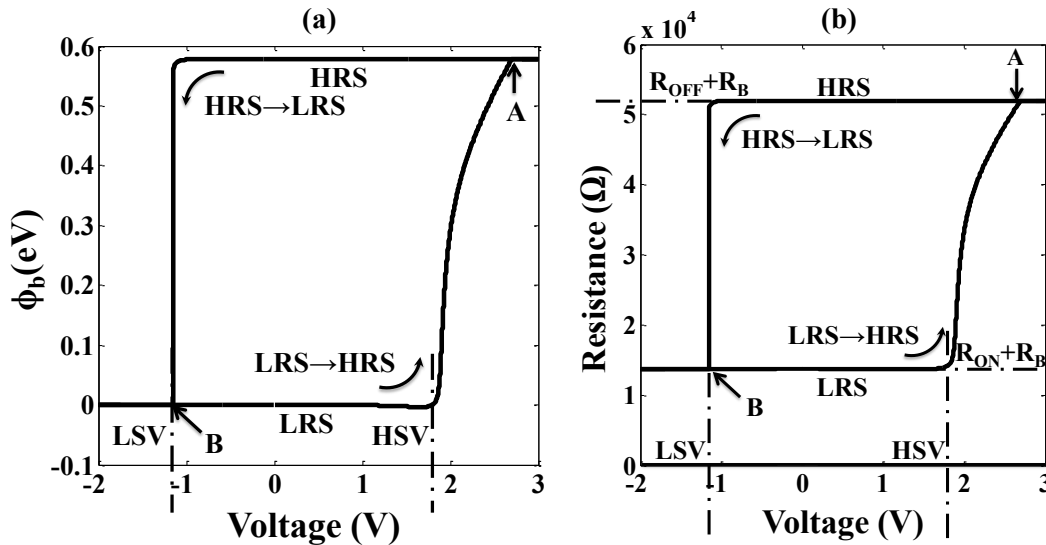


Figure 4.5. The simulation results of (a) The voltage dependence plot of R_{series} and (b) The barrier height ϕ_b against V [21].

[Figure 4.5(a)] and $R_{ON} + R_B$ [Figure 4.5(b)], respectively. These results are in agreement with the physics of the Ta_2O_5/TaO_x RRAM which reflects the inverse proportionality of ϕ_b height and R_{series} to the density of V_o in the doped region (increasing V_o in the filament reduces w). In addition, the dependency of ϕ_b on w and hence, on LSV [Figure 4.5(a)] reflect the intrinsic rectifying effect while at HRS. It is also shown in figures Figure 4.4 and Figure 4.5 that although the bias keeps increasing after the device switch to either state, the parameters , ϕ_b , and R_{series} will not be affected by this increase. Figures Figure 4.5(a) and (b) show that R_{series} and ϕ_b keep the same values after points A and B for HRS and LRS, respectively. Similarly, w remains stable after points A and B (see Figure 4.4). This reflects the self-limiting effect in the model. Also, it can be seen that these three parameters will not change until the opposite polarity switching voltage is reached (LSV and HSV for points A and B, respectively). This shows that the model exhibit the BRS property.

4.5.3. Electric Field Effect

The field evolution with respect to V is shown in Figure 4.6. It can be seen that the field increases and decreases during the stages (HRS→LRS) and (LRS→HRS), respectively. The field evolution with respect to w is presented in the inset of Figure 4.6 which shows that the field reaches E_{LRS} and E_{HRS} at $w = 0$ and $w = 1$, respectively. It is also shown that once the field reaches $E_{HRS→LRS}$ at LSV, it drives $v(t)$ to have significant influence on the nanoscale term w which trigger the abrupt switching property and w switch rapidly to 0. This is associated with an abrupt drop in the current. However, different from the three parameters in section 4.5.2, Figure 4.6 shows that E increases slightly after points A and B (after switching into HRS and LRS). Before the switching occur, E is affected by both, the increase/decrease in w and

the increase in V , following (10). Although w stops changing once the field reaches A or B (see inset of Figure 4.6) and it will no longer affect E , V continues to increase to around 3 and -2 V which further increases the field. The resulted field after B is concentrated on the tip of the doped region only and has no effect on the ions migration. Hence, and as mentioned earlier, this field does not change ϕ_b , and R_{series} .

It can be seen in Figure 4.7(a) that a less abrupt switching behaviour is observed in the I - V characteristic while switching into HRS compared to that of LRS switching [see segment AC]. This behaviour can be further explained by plotting the linear I - V curve during the switching stage (LRS→HRS) together with w - v curve [Figure 4.7(b)]. The three points A–C depicted in Figure 4.7(a) are also shown in Figure 4.7(b) which indicate the switching region. Figure 4.7(b) shows that when a positive bias is ramped and after it exceeds its HSV (correspond to point A on I - V curve), w grows rapidly to around 40% of its total thickness at a decreasing rate (point

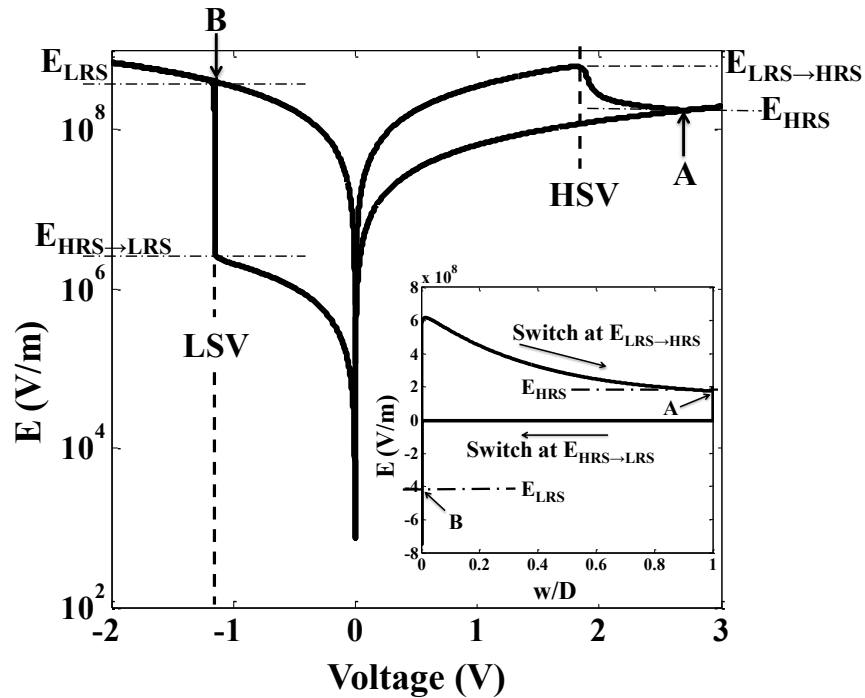


Figure 4.6. Simulated E - V characteristics in semi-log scale plot for the complete evolution of E and (inset) E - w simulation in linear scale [21].

B on I - V curve) before its growth rate continues dropping further at a higher rate for the remaining length (correspond to segment BC in I - V curve). This mechanism is reflected in the proposed model in the sinh dependency of $v(t)$ on the evolution of E . As the doped region length decreases due to oxygen ions migration into Ta_2O_5 layer, E on the increasing length of w keeps dropping, following (10), and strongly slowing down $v(t)$. This behaviour explains the corresponding drop in the current during this switching stage. It also can explain the reason of using a higher RESET voltage compared to the SET process to avoid self-limiting effect due to the small remaining E and to rupture the whole CF during the required time.

The observed small deviation during the switching stage LRS \rightarrow HRS (see Figure 4.2) can be attributed to different possible factors. Some oxygen ions might come from the sides of the

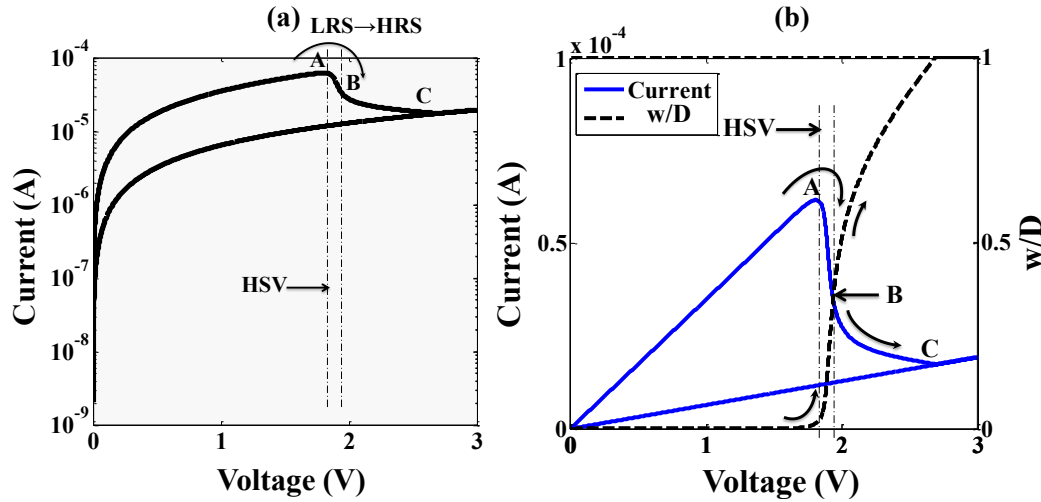


Figure 4.7. (a) Simulation results of I - V curve in semi-log scale plot and (b) Simulated linear I - V and w - V curves for the LRS \rightarrow HRS switching stage [21].

doped region [18] during the RS. Besides that, the ionic drift in the oxides may include a complex interplay of drift, diffusion, and thermophoresis [7].

4.5.4. The Effect of Adding TPF to the RRAM I – V Characteristic Equation

The results of applying the proposed mathematical model to Ta₂O₅/TaO_x bi-layered RRAM physical models with different insulator layer thickness can be perceived by examining Figure 4.8 which shows the I – V characteristics of the proposed model for 3 nm Ta₂O₅ layer together with the experimental results in [17]. The physical model in [17] has the same cell structure as [16] but with a 3 nm Ta₂O₅ layer thickness. The I – V curve is obtained by applying a sinusoidal wave voltage of 5 s period with voltages of -2 and 3 V for the SET and RESET, respectively. Also, since δ in [17] remains in the range (≥ 3 nm), then the value of η is given by $\eta_{D_2=0}$ as in (26). It can be seen that the proposed model showed a good agreement with the experimental results in [17] which further strengthen the assumptions in the proposed model, especially the

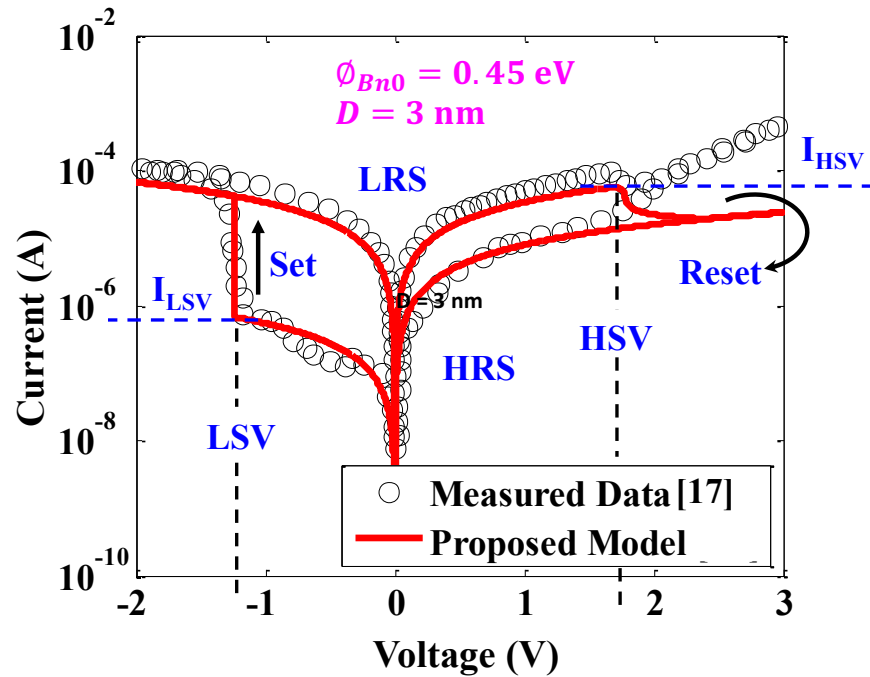


Figure 4.8. Experimental measurements [17] and the semi-log scale plot of the modelling results I – V characteristics with $D = 3$ nm [21].

TPF approximation. Thus, significant improvement to the proposed model is achieved by adding TPF term. When the RRAM model is developed by taking into account the insulator layer thickness and tunnelling current, TPF emphasizes the dependency of the RRAM current values on the physical characteristics of the insulator layer. Without adding TPF, the current equation follows the standard Schottky barrier conduction equation for metal-semiconductor system, which leads to considerably larger values than the corresponding experimental results.

4.5.5. The Agreement of the Proposed Model to the Attributes of the Zero-Crossing Behaviour for the Memristive System

The proposed RRAM model elucidated another important property of the memristive devices identified in [9] and [16] which is the zero-crossing behaviour. This means that, regardless of the RRAM resistance, the frequency of the applied input signal, or the state variable values w , the RRAM output current is always zero when the input voltage reaches zero. As it can be clearly seen in figures Figure 4.2 and Figure 4.8 for the applied periodical input voltages, the attained property is satisfied in the I – V characteristics of the proposed RRAM model, regardless of the values of the three parameters mentioned above.

SPICE MODELLING OF Ta₂O₅/TaO_x Bi-Layered RRAM

Related Publications:

F. O. Hatem, T. N. Kumar, and H. A. F. Almurib, “A SPICE Model of the Ta₂O₅/TaO_x Bi-Layered RRAM,” *IEEE Transactions on Circuits and Systems I: Regular Papers*, vol. 63, no. 9, pp. 1487-1498. 2016.

Summary

Designing a SPICE model is a critical step toward understanding the behaviour of the RRAM devices when integrated in memory design for the future generation storage devices. In this chapter, a SPICE model is developed for the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM. The proposed model emphasizes the impact of the change in the switching layer thickness on the device behaviour at LRS, HRS, and the transitional period. The validity of the proposed model is verified through using three different sets of experimental data from $\text{Pt}/\text{Ta}_2\text{O}_5/\text{TaO}_x/\text{Pt}$ RRAM with switching layer thickness smaller than 5 nm. The SPICE model reproduced all the major features from the experimental results for the SET and RESET processes and also the asymmetric and the symmetric characteristics in HRS and LRS, respectively. The proposed SPICE model matches the measured experimental results with an average error of $< 11\%$ and a maximum error of $< 70\%$. It also showed stable behaviour for its HRS and LRS regions under different types of input signals. The model is parameterized in order to fit into $\text{Ta}_2\text{O}_5/\text{TaO}_x$ RRAM devices with switching layer thickness smaller than 5 nm, thus, facilitating the model usage. The model can be included in the SPICE-compatible circuit simulation and is suitable for the exploration of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM device performance at circuit level. The obtained simulation results show that the proposed SPICE model can successfully demonstrate four intrinsic features extracted from the experimental observations of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ RRAM in which the first three features are related directly to the change in D . 1) The model is first verified that it can produce the correct I - V behaviour when D is changed from 4 to 3 nm. 2) The model is then proved that it can demonstrate the dependency of the HSV on D where HSV is the required voltage for the device to switch into HRS. 3) The ability of the SPICE model to demonstrate the effect of changing D on its LRS and HRS is also

explored. 4) The model is examined and verified that it can successfully capture the temporal increase in the HRS during SET switching; an important intrinsic feature of the P/Ta₂O₅ interface which has been reported in [1]. To further verify the validity of the proposed SPICE model, pulse switching simulation with different RESET pulse amplitudes is conducted. The simulation results match with the measured data and show that the model can successfully demonstrate the change in the current with regards to RESET pulse amplitude. Also, the SPICE model is tested for predicting the correct RS behaviour for different types of the conventional voltage signals. The proposed model provided full RS switching with the same LRS and HRS value despite the type of the stimulus signal. As a final verification step, the integration capability of the proposed SPICE model with the CMOS technology is tested by simulating a non-volatile D-Latch circuit.

To the best of the researcher's knowledge, this is the first Ta₂O₅/TaO_x bi-layered RRAM physics-based model that has been implemented as SPICE subcircuit, correlated to more than one thickness, successfully verified using the above intrinsic features, and proved to show a stable behaviour for sinusoidal, rectangular, and triangular inputs. This SPICE model can be used for the bi-layered RRAM-based circuit applications, providing more flexibility in the used device thickness and the bias signal. The proposed model can be considered as a first step approach into finding a more universal SPICE model that can predict the behaviour of the bi-layered RRAM devices with different oxide materials and thicker switching layers (thicker than 4 nm).

5.1. The Structure of the Proposed Model and its Bipolar Resistive Switching Mechanism

The structure of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM SPICE model is shown in Figure 5.1 (adapted from the RRAM mathematical model in chapter 4). The BRS mechanism is similar to that of the mathematical model where the TaO_x layer is highly doped with oxygen vacancies (V_o) and its resistance is assumed to be R_B . D is the thickness of the Ta_2O_5 layer and its resistance R_I .

Low Resistance State: LRS is reached when a negative voltage is applied as in Figure 5.1(a). In this case, oxygen ions in the Ta_2O_5 layer and in the vicinity of the interface region will be pushed toward TaO_x layer, leaving behind donor-like oxygen vacancies which dope the Ta_2O_5 layer [1], [21]. This results in a metal rich doped region and reduces the barrier height ϕ_b , simultaneously [21]. When all the length of CF in the Ta_2O_5 layer is doped ($w=0$), the device

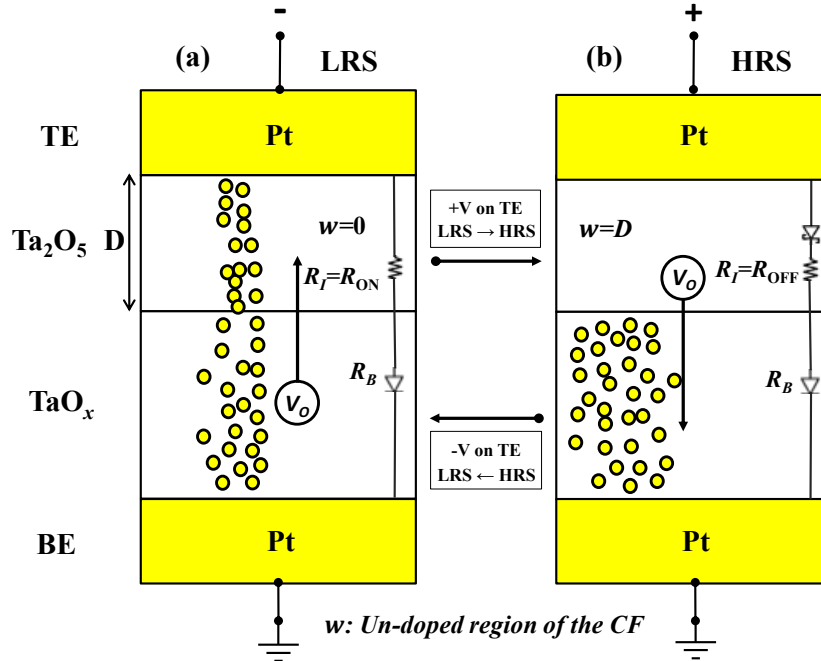


Figure 5.1. A schematic representation of the proposed SPICE model and its switching mechanism. (a) The LRS and (b) the HRS [37].

reaches its LRS and the Schottky-like interface between TE and Ta₂O₅ is changed into ohmic [21]. This is shown in Figure 5.1(a).

High Resistance State: When a positive voltage is exerted [Figure 5.1(b)], oxygen ions migrate from the bulk layer toward Ta₂O₅ layer and the interface region (the oxygen vacancies are repelled away from Ta₂O₅ layer) which un-dope the Ta₂O₅ layer and increases the barrier height (the ohmic interface is changed back to Schottky-like interface). Consequently, the CF in the Ta₂O₅ layer is un-doped ($w=1$). This state change is indicated in Figure 5.1(b).

Table 5-1. The equations used in the proposed SPICE RRAM model, extracted from the RRAM mathematical model in chapter 4 [37].

Modelling of the Un-Doped Region of the CF Evolution	
$\frac{dw}{dt} = v(t) \approx \begin{cases} v_{1,2} \cdot a \cdot c \cdot \exp(-\frac{U}{KT}) \cdot \sinh \frac{x_{1,2}E}{E_0}, & 0 < w < D \\ 0, & 0 \geq w \geq D \end{cases}$	(1)
$E = \frac{V_U}{w} = \frac{V_D}{w + R_r(D - w)}$	(2)
$V_D = V - IR_B - V_S$	(3)
$V_D = \left(R_{ON} \left(1 - \frac{w}{D}\right) + R_{OFF} \cdot \frac{w}{D}\right) \cdot I = R_I \cdot I$	(4)
$V_S = V - I(R_{series})$	(5)
Mathematical Modelling of the I - V Behaviour and the Temperature	
$I = AA \cdot T_0^2 \exp^{-(n_{1,2}\phi_b)/V_T} \left(\exp^{\frac{V_S}{\eta V_T}} - 1 \right) \left(\exp^{-\sqrt{\xi} w \times 10^{10}} \right)$	(6)
$\eta = m[(\eta_{LRS})(1 - \frac{w}{D}) + (\eta_{HRS})\frac{w}{D}]$	(7)
$\phi_b = \phi_{Bn} - \Delta\phi = \phi_{Bn0} \left(\frac{w}{D}\right) - \left[\frac{q^3 N \phi_s}{8\pi^2 \epsilon_s^3}\right]^{1/4}$	(8)
$T = T_0 + I^2 \cdot R_I \cdot R_{th}$	(9)

5.2. SPICE Model Implementation

The complex mechanisms of w evolution and the current conduction are summarized in the related equations (1)–(9) in Table 5-1 and have been implemented in LTSPICE as a single Pt/Ta₂O₅/TaO_x/Pt device. Table 5-2 includes the parameters used in SPICE simulation with their values. The structure of the SPICE model is shown in Figure 5.2 which determines the single device time-dependent current flow at LRS, HRS and the transitional state. The equivalent SPICE subcircuit implementation of this structure is shown in the listing in Figure 5.3.

Table 5-2. Parameters Used in the proposed SPICE RRAM model simulation for $D = 4$ nm and 3 nm [37].

Parameter	Value When ($D = 4$ nm / 3 nm)	SPICE Model Symbol
T_0	300 K	T0
D	4 nm [16], [21] / 3 nm [17], [21]	D
V_T	26 mV	VT
A	$9 \times 10^{-6} \text{ cm}^2$ [16], [21]	Ar
ε_s	$27 \times \varepsilon_0$	es
ε_0	$8.85 \times 10^{-12} \text{ F} \cdot \text{m}^{-1}$	e0
U	1 eV [18]	U
a	1 nm [18], [67]	a
k	$1.38 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$	k
q	$1.6 \times 10^{-19} \text{ C}$	q
A^*	$120 \times 10^4 \text{ A} \cdot \text{m}^{-2} \cdot \text{K}^{-2}$ [32]	As
N	$1 \times 10^{23} \text{ C} \cdot \text{m}^{-3}$	N
ξ	0.00175 / 0.0031	Phi_T
R_{OFF}	40 k Ω / 20 k Ω	Roff
R_{ON}	1.7 k Ω	Ron
R_B	12 k Ω	Rb
c	$1 \times 10^{13} \text{ Hz}$ [67]	f
ϕ_{Bn0}	0.6 eV [16], [21] / 0.45 eV	Phi_Bn0
x_1	215 / 95	x1
x_2	0.4 / 0.03	x2
v_1	1	v1
v_2	0.6e-6	v2
n_1	0.1852 / 0.1905	n1
n_2	0.0117	n2
m	6e6	m

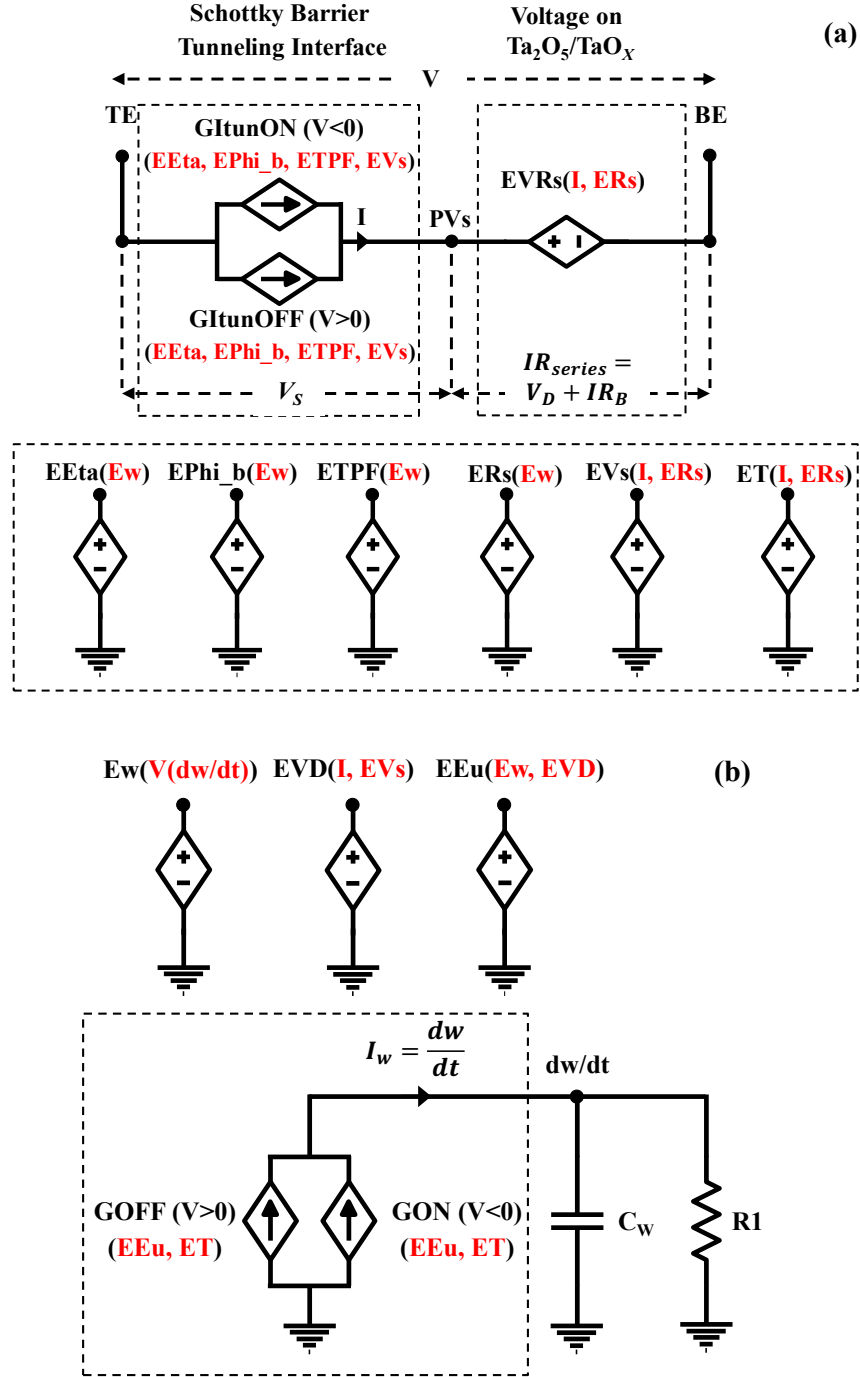


Figure 5.2. LTSPICE implementation of the proposed SPICE model. (a) The two terminal (current path) SPICE implementation of the single Pt/Ta₂O₅/TaO_x/Pt device and the implementation of the related parameters ϕ_b , η , TPF, and V_s . (b) The SPICE subcircuit implementation of w evolution, E , and the self-limiting effect [37].

```

00 .SUBCKT Ta2O5_RRAM plus minus TPF Phi_b Vs PARAMS:
01 +T0=300 D=4e-9 VT=0.0258 Ar=9e-10 e0=8.85e-12 U=1 a=1e-9
02 +k=1.3806e-23 q=1.60217e-19 As=120e4 es=27*e0 N=1e23
03 +Phi_T=0.00175 Roff=40k Ron=1.7k Rb=12k Rth=1e8 f=1e13
04 + Phi_Bn0=0.6 x1=215 x2=0.4 v1=1 v2=0.6e-6 n1=0.1852
05 +n2=0.0117 m=6e6
      *****Current Path SPICE Subcircuit*****
06 EV V 0 value={V(plus)-V(minus)}
07 EPhi_Bn Phi_Bn 0 value={ Phi_Bn0 *V(w)/D}
08 ED_Phi D_Phi 0 value={(((q**3)*N*V(Phi_Bn))/(8*(pi**2))*
09 +(es**3))**0.25}
10 EPhi_b Phi_b 0 value={V(Phi_Bn)-V(D_Phi)}
11 EEta Eta 0 value={m*((10*(D-V(w))/D)+(9*V(w)/D))}
12 ETPF TPF 0 value={exp(-V(w)*sqrt(Phi_T)* 1e10)}
13 ERs Rs 0 value={Rb+(Ron*(D-V(w))/D)+(Roff*V(w)/D)}
14 EVRs PVs minus value={V(Rs)*I(EVRs)}
15 EVs Vs 0 value={V(V)-(I(EVRs)*V(Rs))}
*****Device Current when (V<0)*****
16 ElsOn IsOn 0 value={stp(-V(V))*Ar*As*(T0**2)*
17 +exp(-n1*V(Phi_b)/(k*T0/q))}
18 GitunON plus PVs value={V(IsOn)*(exp(V(Vs)/(V(Eta)*VT))-
19 +1)* V(TPF)}
*****Device Current when (V>=0)*****
20 ElsOff IsOff 0 value={stp(V(V))*Ar*As*(T0**2)*
21 +exp(-n2*V(Phi_b)/(k*T0/q))}
22 GltunOFF plus PVs value={(-V(IsOff))*
23 +(exp(-V(Vs)/(V(Eta)*VT))-1)*V(TPF)}
***** w and E Evolution Dynamics *****
24 EVD VD 0 value={V(V)-(I(EVRs)*Rb)-V(Vs)}
25 EEu Eu 0 value={V(VD)/(V(w)+((Ron/Roff)*(D-V(w))))}
26 ET T 0 value={T0+(Rth*(I(EVRs)**2)*(V(Rs)-Rb))}
27 EKT KT 0 value ={k*V(T)}
*****Dynamical ON switching (V<0)*****
28 Ewset wset 0 value={v1*a*f*exp(-U*q/V(KT))}
29 GON 0 dw/dt value={V(wset)*sinh(stp(-V(V))*
30 +(x1*q*a*V(Eu))/V(KT))}
*****Dynamical OFF switching (V>=0)*****
31 Ewreset wreset 0 value={ v2*a*f*exp(-U*q/V(KT))}
32 GOFF 0 dw/dt value={V(wreset)*sinh(stp(V(V))*
33 +(x2*q*a*V(Eu))/V(KT))}
34 Cw dw/dt 0 1 IC=0
35 R1 dw/dt 0 1e9MEG
36 Ew w 0 value='((V(dw/dt) > 0) & (V(dw/dt) < D)) ?
37 +{V(dw/dt)} : {V(dw/dt) <= 0 ? {0} : {D}}'
38 .end Ta2O5_RRAM

```

Figure 5.3. LTSPICE subcircuit implementation of the proposed bi-layered RRAM SPICE model [37].

5.2.1. Current Path SPICE Subcircuit

It can be seen in Figure 5.2(a) and the listing in Figure 5.3 that the single $\text{Ta}_2\text{O}_5/\text{TaO}_x$ RRAM device is represented by the two terminals SPICE subcircuit. The current port equation of the subcircuit is composed of two elements connected in series as shown in the top part of Figure 5.2(a). The Schottky barrier tunnelling element (the upper-left corner of Figure 5.2(a) and code lines 15–23) contains a parallel connection of two voltage-controlled current sources (VCCS) GItunON and GItunOFF (G-type source in LTSPICE) which model the tunnelling current when $V < 0$ (code lines 16–19) and $V > 0$ (code lines 20–23), respectively. The correct VCCS is selected by using the applied bias V (code line 6) as a parameter in the STP function in code lines 16 and 20. In this case, GItunON will be delivering a charge into the point PVs when $V < 0$ whereas GItunOFF is activated when $V > 0$. The function STP(x) is a unit step that returns 1 and 0 for $x \geq 0$ and $x < 0$, respectively. The current I passing through the point PVs is the total current through the RRAM device as given by (6). The expression for the reverse bias condition GItunOFF is similar to GItunON except that the polarity of Schottky potential and the current direction are reversed. The voltage drop V_S on the tunneling element represents Schottky barrier voltage as shown in Figure 5.2(a). The second element in the port equation (the upper-right corner of Figure 5.2(a) and code line 14) is a voltage-controlled voltage source (VCVS) EVRs (E-type source in LTSPICE) which represents the total voltage drop on the device (IR_{series} or $V_D + IR_B$) except that of V_S where V_D is given in code line 24. However, in order to produce the total output current I from GItunON and GItunOFF, four parameters ϕ_b [given by (8)], η [given by (7)], TPF [given by (6)], and V_S [given by (5)] are modeled using VCVSs: EPhi_b (line 10), EEta (line 11), ETPF (line 12), and EVs (line 15), respectively. The

terminal voltage of the first three voltage sources is controlled by the instantaneous value of w . The value of w is produced using the VCVS E_w [Figure 5.2(b)] which is discussed in the next section. The forth VCVS source E_v is implemented based on the device current and the value of R_{series} . The resistance R_{series} is implemented as ERs as shown in Figure 5.2(a) and code line 13.

It can be seen that the proposed SPICE model depends mainly on VCVSs instead of the same parameters values being lumped directly into different locations in the SPICE listing. This portability makes it easy to modify any of these parameters for future enhancements. Also, it allows the use of these parameters in the external circuit (for further analysis of the model) by adding extra output pin (e.g. TPF in code line 01). The rest of the code in the first part of the listing is explained as follows. In lines 1–5, the model simulation parameters are defined which can be changed based on the physical device. Code lines 7 and 8 correspond to ϕ_{Bn} and $\Delta\phi$, respectively which are used to obtain ϕ_b in code line 10.

5.2.2. w and E Evolution Dynamics SPICE Subcircuit

In the second part of the SPICE listing, code lines 24–37 depict the implementation of the circuit structure in Figure 5.2(b) which includes the modelling of w and E evolution dynamic. In lines 24 and 25, two VCVS, E_{Eu} and E_{VD} are used to calculate E based on V_D as in (2) and (3). E_{Eu} is used in lines 28–33 to implement two VCCSs, G_{ON} and G_{OFF} which are used to produce the current $I_w = \frac{dw}{dt}$ using (1) [see Figure 5.2(b)]. Based on the applied bias polarity, the function STP is used to switch-on G_{ON} ($I_w = G_{\text{ON}}$) when $V < 0$ (switching into LRS)

while GOFF is used ($I_w = \text{GOFF}$) when $V > 0$ (switching into HRS). Code lines 36 and 37 implement a VCVS E_w which is used to calculate the instantaneous value of w . This is achieved by integrating I_w inside a nested ternary function. The integration is performed by taking the voltage $V(dw/dt)$ across the capacitor C_w [see Figure 5.2(b)]. The capacitor C_w has a value of 1 F in order to keep the units of w unchanged (in nanometer). The nested ternary function is also used to model the self-Limiting effect of the device as in (1). The first ternary expression checks if w is still within the physical allowable region of $(0-D \text{ nm})$. If this is the case, E_w keeps changing (increasing or decreasing), following the voltage on C_w otherwise, another nested ternary function is implemented to account for the self-limiting effect. In the second ternary function, the first and second conditions in the IF clause guarantee the correct w thickness limitation when switching into LRS (True IF clause) and HRS (False IF clause), respectively. The initial state of the device is assumed to be in the ON states. This is implemented in line 34 by setting the initial voltage on C_w to 0 and hence, initial w value is also 0 nm. Furthermore, in order for the simulation to determine the initial DC operating point, a dc path from point dw/dt to the ground is provided using a resistor R1 with a very large value as in code line 35.

5.3. Model Evaluation and Simulation Studies

5.3.1. The Agreement with the I – V Characteristics for Different Values of D

The validity and the quality of the SPICE model are first verified by comparing the obtained simulation results in LTSPICE with the experimental data from Pt/Ta₂O₅/TaO_x/Pt RRAM devices with $D = 4$ and 3 nm where D is decided during the device fabrication process (by more

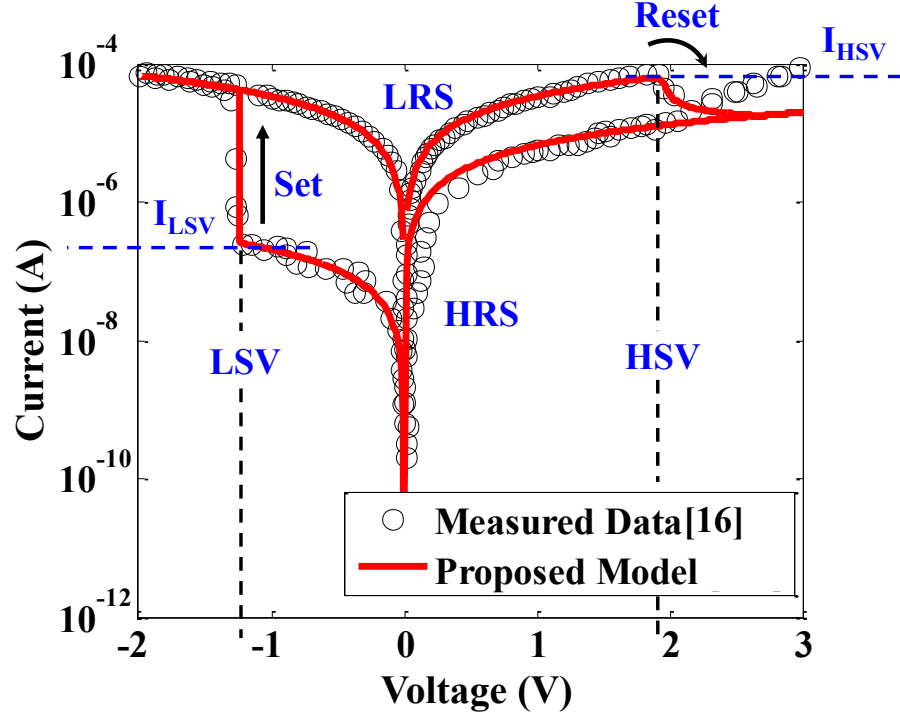


Figure 5.4. Experimental measurements [16] and the semi-log scale plot of the SPICE model simulation I - V characteristics with $D = 4$ nm, $\phi_{Bn0} = 0.6$ eV, $\xi = 0.00175$ eV, $R_{OFF} = 40$ k Ω , $x_1 = 215$, $x_2 = 0.4$, $n_1 = 0.1852$, and a -2/3 V 100 Hz sine wave bias signal [37].

or less oxidation) [8]. Using the subcircuit in Figure 5.2 and the associated parameters adjusted in Table 5-2, Figure 5.4 shows the semi-log scale simulated I - V characteristics for the SPICE model (solid line) and the experimental data from [16] for $D = 4$ nm. The simulated and the experimental data in Figure 5.4 are obtained using the same bias protocol of a 100 Hz sine wave, SET voltage of -2 V and 3 V RESET voltage. The model simulation results match with the measured data and show excellent agreements, both qualitatively and quantitatively except for a small discrepancy in the simulated current magnitude while switching into HRS. The deviation has been explained in the previous chapter and attributed to the ..It is observed that $LSV = -1.24$ V, $I_{LSV} = 0.25$ μ A, $HSV = 1.9$ V, and $I_{HSV} = 70$ μ A. I_{LSV} and I_{HSV} are the device current at LSV and HSV, respectively.

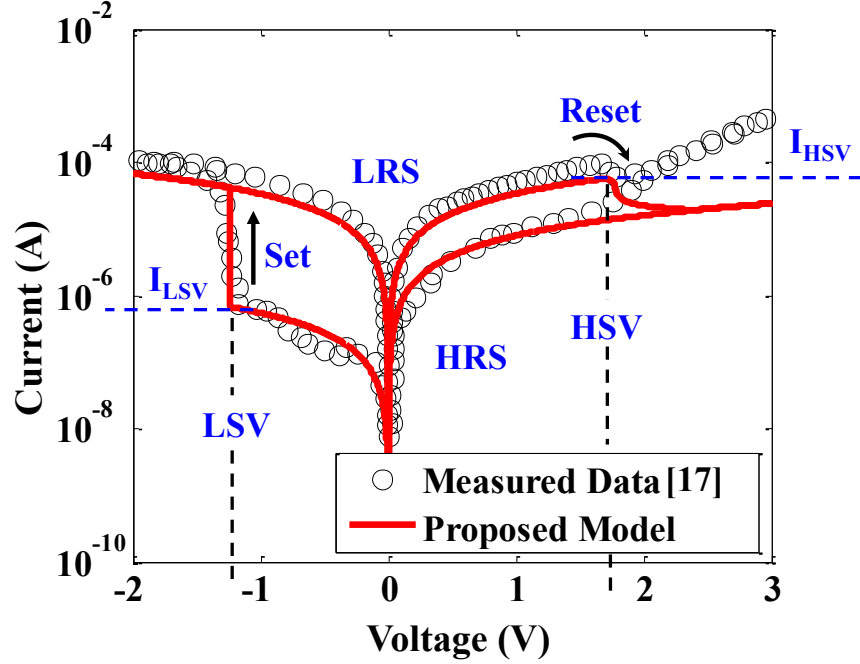


Figure 5.5. Experimental measurements [17] and the semi-log scale plot of the SPICE model simulation I - V characteristics with $D = 3$ nm, $\phi_{Bn0} = 0.45$ eV, $\xi = 0.0031$ eV, $R_{OFF} = 20$ k Ω , $x_1 = 95$, $x_2 = 0.03$, $n_1 = 0.1905$, and a $-2/3$ V 0.2 Hz sine wave bias signal [37].

To further verify the correctness of the SPICE model, the proposed model is used to reproduce the I - V characteristics from the experimental data with smaller Ta₂O₅ layer thickness ($D = 3$ nm) [17]. However, due to the change in the Ta₂O₅ layer thickness and hence, its resistance at HRS, some of the used parameters must be tuned to reflect this change as follows. It is assumed that ϕ_{Bn0} is reduced compared to its initial height when $D = 4$ nm, following the reduction in the insulating volume where the smaller insulating volume results in smaller band gap [17], [68]. Thus, ϕ_{Bn0} is approximated to be reduced by around 25% to $\phi_{Bn0} \approx 0.45$ eV, following (8) which is similar to the value used in [17] ($\phi_{Bn0} = 0.4$ eV for $D = 3$ nm). Besides the change in ϕ_{Bn0} , changes will occur to R_{OFF} , X_1 , X_2 , ξ , and n_1 in which $R_{OFF} = 20$ k Ω s, $X_1 = 95$, $X_2 = 0.03$, $\xi = 0.0031$, and $n_1 = 0.1905$. The simulation results of applying the proposed model into Ta₂O₅/TaO_x RRAM with $D = 3$ nm is shown in Figure 5.5. The measured and calculated

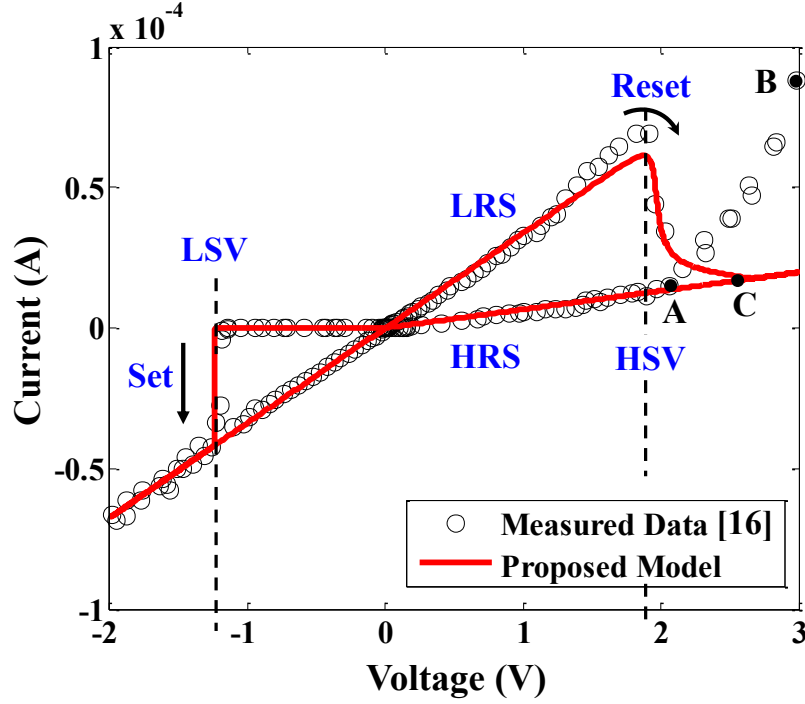


Figure 5.6. Experimental measurements [16] and the linear scale plot of the SPICE model simulation I - V characteristics with $D = 4$ nm, $\Phi_{Bn0} = 0.6$ eV, $\xi = 0.00175$ eV, $R_{OFF} = 40$ k Ω , $x_1 = 215$, $x_2 = 0.4$, $n_1 = 0.1852$, and a $-2/3$ V 100 Hz sine wave bias signal [37].

I - V curves in Figure 5.5 are obtained by applying a sine wave voltage of 5 s period with voltages of -2 and 3 V for the SET and RESET, respectively. It can be seen that the simulation results in Figure 5.5 are consistent with the experimental data which shows that the model emphasizes the dependency of the device behaviour on the change of D . This dependency is achieved by integrating the physics involved when D is changed (i.e. integrating D and/or w into E , Φ_b , TPF, and η), providing that D is still within the allowable range for tunneling. It can be seen that $LSV = -1.24$ V, $I_{LSV} = 0.67$ μ A, $HSV = 1.7$ V, and $I_{HSV} = 70$ μ A. The reduction in the HSV value compared to the value obtained when $D = 4$ nm is explained in details in the next section. In addition to the semi-log scale plot of the proposed SPICE model, Figure 5.6 presents the linear I - V characteristics for the device in Figure 5.4.

5.3.2. The Dependency of HSV and LSV on D

Figure 5.7 shows the SPICE model simulation results for $D = 3$ and 4 nm plotted together. These results have already been verified with the experimental data in figures Figure 5.4 and Figure 5.5. By comparing the two devices characteristic, it can be seen that the SPICE model can capture the change in the HSV which decreases for the 3 nm device compared with that of

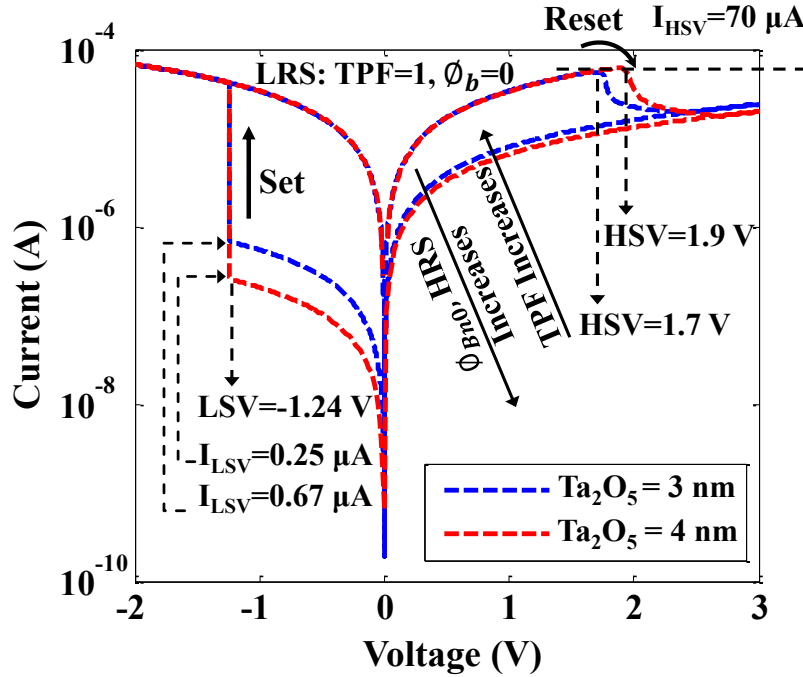


Figure 5.7. The semi-log scale plot of the SPICE model simulation I - V characteristics with $D = 3$ nm, $\phi_{Bn0} = 0.45$ eV (blue line) and $D = 4$ nm, $\phi_{Bn0} = 0.6$ eV (red line). Both curves are obtained using $-2/3$ V Hz sine wave bias signal with 0.2 Hz (for $D = 3$) and 100 Hz (for $D = 4$) [37].

4 nm from around 1.9 V to 1.7 V. Knowing that HSV is the required voltage for E to reach $E_{LRS \rightarrow HRS}$, the SPICE model can capture the change in HSV as follows. When a positive RESET bias is applied and before HSV is reached, E follows (10) and hence, two factors are contributing to the value of E at this stage, D and V_D . Due to the nanoscale nature of the term D in (10), a reduction of D by 1 nm will have a great influence on E_{LRS} . Hence a smaller

voltage V is required to reach $E_{\text{LRS} \rightarrow \text{HRS}}$ when D is reduced from 4 to 3 nm, which explain the smaller HSV obtained in Figure 5.7. It can be seen in Figure 5.7 that during LRS, the parameters TPF and ϕ_b maintain their maximum and minimum values (1 and around 0, respectively), irrespective of the value of D . Thus, HSV is not affected by these two parameters when D is changed.

$$E_{\text{LRS}} = \frac{V_D}{R_T D} = \frac{V - IR_B - V_S}{R_T D}. \quad (10)$$

Besides HSV, the SPICE model can also demonstrate the correct LSV when D is changed. According to the experiments in [8], [17], and [16] (see figures Figure 5.4 and Figure 5.5), the Ta₂O₅/TaO_x RRAM maintains its LSV despite the change in D . Figure 5.7 shows that the SPICE model simulation captures this intrinsic feature and show the same LSV when D is changed from 3 to 4 nm. These results verify that due to the correct modelling of E in (2) and (3), the SPICE model can successfully demonstrate the dependency of HSV and LSV on D .

5.3.3. The Effects of Changing D on the Values of LRS and HRS

The SPICE model can successfully demonstrate the change in LRS and HRS values when D and the value of R_{OFF} are changed. According to the experiments in [8], [17], and [16] (see figure. Figure 5.4 and Figure 5.5), the HRS for Ta₂O₅/TaO_x RRAM decreases by decreasing D while the LRS is insensitive to the change in D . Figure 5.7 shows that the SPICE model can successfully capture this feature where HRS is lowered when D is decreased from 4 to 3 nm whereas LRS remains unchanged. The SPICE model can predict this intrinsic phenomenon as follows.

HRS: While at HRS, the device resistance is determined by $R_B + R_{\text{OFF}} + V_S/I$ [21]. The interface resistance V_S/I at HRS is influenced by TPF and ϕ_b . At HRS, TPF and ϕ_b are proportional to $w = D$ [(6) and (8)] where decreasing D results in larger and smaller values of TPF and ϕ_b (ϕ_{Bn0} is smaller), respectively. As a result, I is increased according to (6) and the interface voltage V_S is decreased (5). Consequently, the resistance V_S/I is reduced for smaller D . Besides V_S/I , R_{OFF} is also reduced for smaller D (due to the smaller insulating volume). It is found that $R_{\text{OFF}} = 20 \text{ k}\Omega$ s provides the best fitting to the experimental results when $D = 3 \text{ nm}$. Therefore, the reduction in V_S/I and R_{OFF} when D is reduced leads to smaller HRS. However, the resistance R_B is insensitive to the change in D .

LRS: Following the same explanation for HRS, the device resistance at LRS is determined by: $R_B + R_{\text{ON}} + V_S/I$. TPF and ϕ_b at LRS have the values of 1 and around 0, respectively, regardless of the value of D (see Figure 5.7) which makes the resistance V_S/I at LRS insensitive to these two parameters (V_S/I reaches its minimum value at LRS). Also, R_B and R_{ON} are selected to satisfy the condition $R_B \gg R_{\text{ON}}$ as in [1]. Hence, the small change in R_{ON} due to the change of D is negligible (R_{ON} is assumed to be fixed in the SPICE model) and the total current while at LRS is limited by the relatively large R_B . This explains why the change in D has no effect on the LRS. These results show that by integrating TPF and ϕ_b , the proposed SPICE model can manifest the dependency of LRS and HRS on D .

5.3.4. The Intrinsic Schottky Barrier and its Effect on the HRS During SET Switching

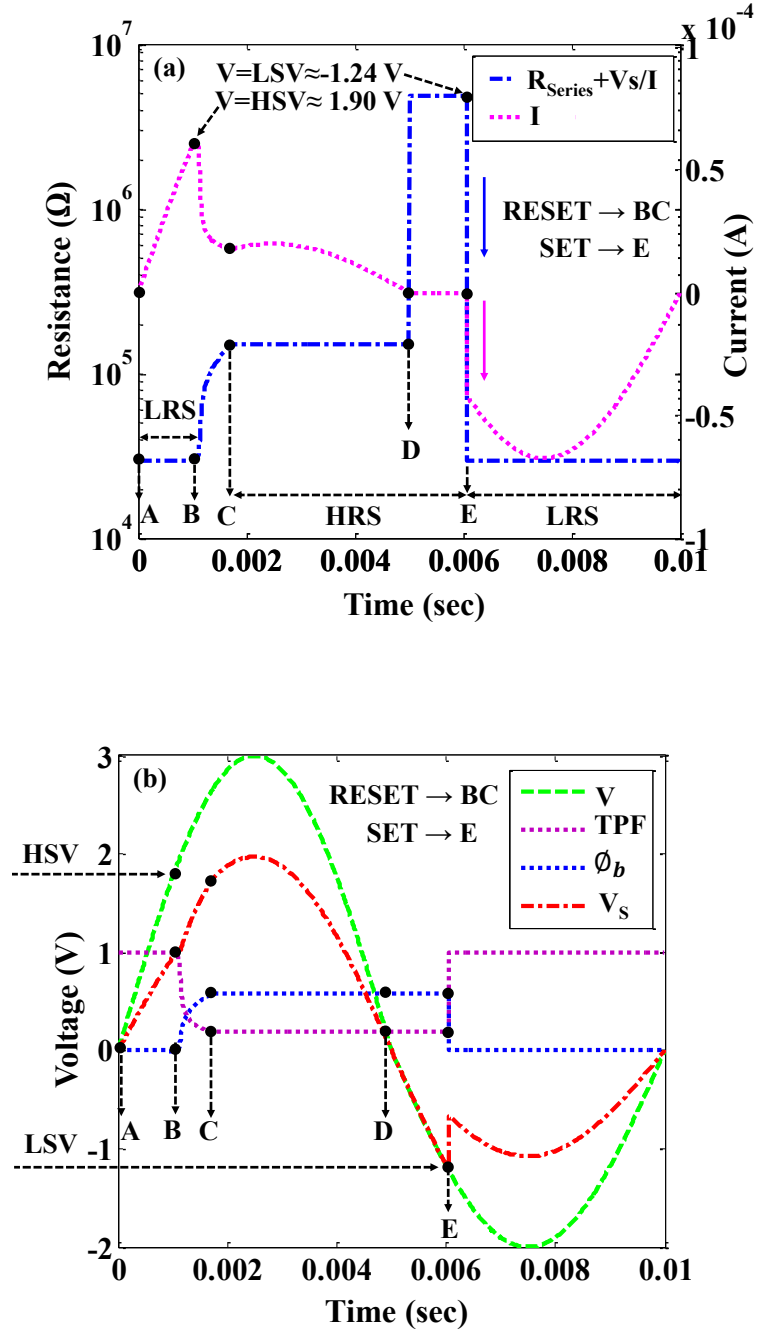


Figure 5.8. (a) The SPICE model simulation of the device total resistance $R_{\text{series}} + V_s/I$ (blue line) and the total current I (purple line) as a function of time for the 4 nm Ta_2O_5 layer thickness and $\phi_{\text{Bn0}} = 0.6$ eV. The curves plotted are obtained for a complete RS cycle using $-2/3$ V 100 Hz sine wave bias signal (b) The corresponding variation in ϕ_b , TPF, V_s , and V [37].

Using the proposed SPICE model, a comprehensive analysis and simulation of Schottky-like tunnelling interface (Pt/Ta₂O₅) reveal that the device resistance during HRS is not fixed, but depends on the bias polarity.

Figure 5.8(a) shows the simulated device resistance $R_{\text{series}} + V_S/I$ and the current I as a function of time for $D = 4$ nm for a complete RS cycle while

Figure 5.8(b) compares the corresponding variation in ϕ_b , TPF, V_S , and V . Assuming LRS as the initial state (point A), it can be seen that the device first starts switching into HRS when HSV=1.9 V is reached (point B). The device reaches its HRS at the end of the switching period (end of BC). However, the imperative remark that can be observed is that once a negative SET bias is applied (point D), the resistance switches from few hundreds of Kilo Ohms (HRS value) to few Mega Ohms and the current tends to align with 0 A. The device maintains this very high resistance until LSV=-1.24 V is reached (point E) where the resistance drops significantly and an abrupt increase in the current is observed, indicating LRS. This behaviour is attributed to the coexistence of the reversed-biased Schottky barrier associated with TPF as explained next. The device current is determined by the multiplication of three terms T1, T2, and TPF as follows:

$$I = \underbrace{AA \cdot T_0^2 \exp^{-(\phi_b)/V_T}}_{T1} \underbrace{\left(\exp^{\frac{V_S}{\eta V_T}} - 1 \right)}_{T2} \underbrace{\left(\exp^{-10^{10} \times \sqrt{\xi} w} \right)}_{TPF}. \quad (11)$$

1) While at LRS (AB), I is mainly influenced by T2 and varies according to V . TPF equals 1 and has no effect on suppressing I at LRS (no tunneling current). Similarly, $\phi_b \approx 0$ at LRS (ohmic contact) and T1 is fixed at its maximum value and does not reduce I . **2)** Overtime, HSV

is reached (point B), RESET starts, and all the three terms in (11) will have a great influence on I during the switching. TPF starts to decrease; reducing I (indicates tunneling). Eventually, TPF switches to its minimum value at $w = D$ (point C). Simultaneously, ϕ_b is ramped to its maximum value at $w = D$ (point C) and tunneling Schottky barrier is formed. **3)** While the device is at HRS, I at the positive bias region (CD) is suppressed by means of TPF and a forward biased tunnelling Schottky barrier (positive V_S) composed of T1×T2 where $T2 \geq 0$. In contrast, I at the negative bias region (DE) is suppressed by the same value of TPF and T1 but with Schottky barrier in T2 being reversed biased (negative V_S) where $T2 \leq 0$. As a result, I in segment DE is getting closer to zero compared to that in the segment CD because $|T2|$ is smaller for negative V_S compared to positive V_S [$(\exp^y - 1)$ is smaller for negative y]. Consequently, the very small I forces V_S/I and the total resistance ($R = R_{\text{series}} + V_S/I$) to switch to the temporal high value observed in

Figure 5.8(a). **4)** Once LSV is reached (point E), ϕ_b drops to 0 eV (the contact is changed into Ohmic), forcing T1 to increase considerably. This is associated with TPF increases again to 1. The increase in T1 and TPF eliminate the effect of reverse biased Schottky barrier in T2 and hence, I increases again which in turn forces V_S/I to drop to its minimum value and LRS is reached. These results show that the proposed SPICE model can successfully capture the asymmetric current profile at HRS and highlight the dependency of the HRS on the bias polarity, making the model more reliable and predictive for potential circuit application.

5.3.5. Testing the Model under Different Types of Input Signals

The use of the conventional voltage quantities (e.g. sinusoidal, rectangular, and triangular waveforms) is common in many potential memory applications. Therefore, in order to increase the number of the bi-layered RRAM-based circuit applications, a SPICE model that has a stable behaviour (same levels of LRS and HRS) under changing its input stimulus type is essential (providing the input signal is large enough to provide the required LSV and HSV). After the proposed SPICE model matches the experimental results for a sinusoidal signal, it is tested under the same -2 V SET and 3 V RESET voltages but for a triangular and rectangular signals

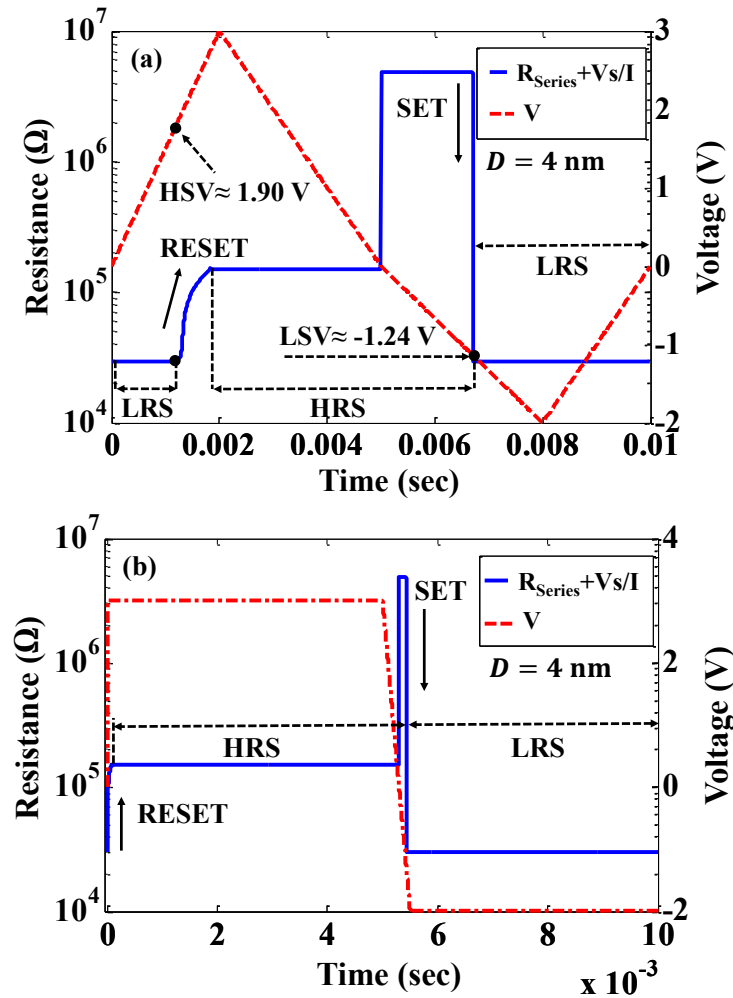


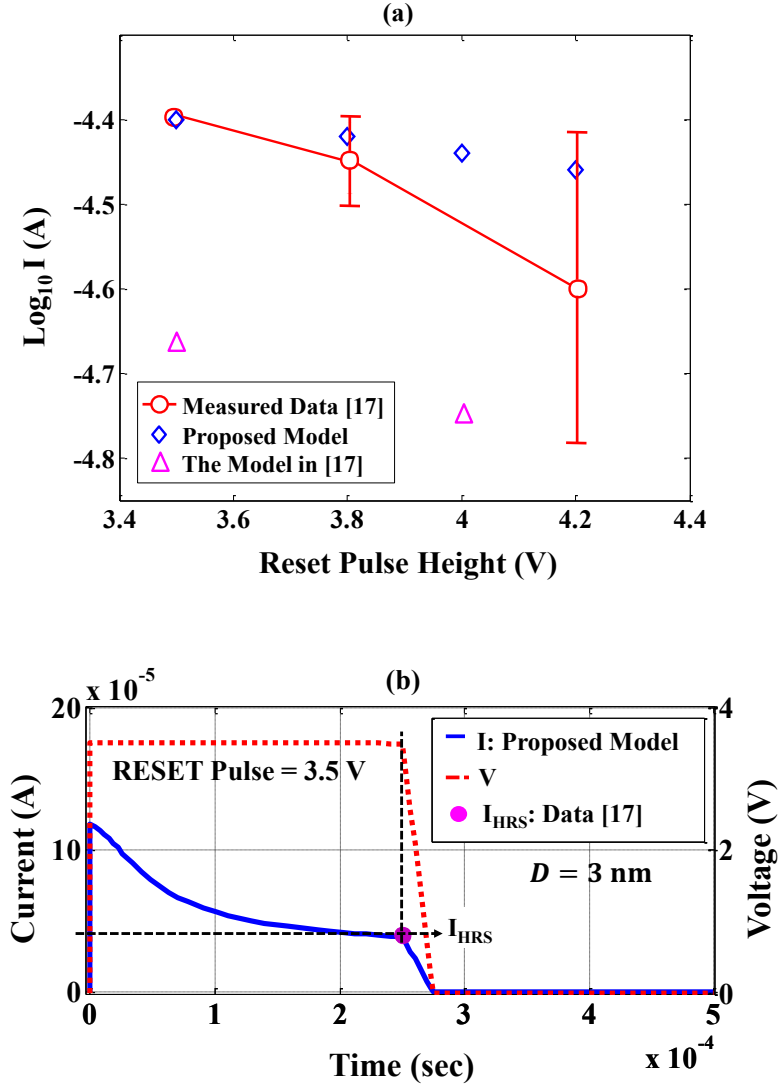
Figure 5.9. The SPICE model simulation of the device total resistance $R_{series} + V_S/I$ (blue line) and the applied voltage V (red dashed line) as a function of time for $D = 4$ nm. The curves plotted are obtained for a complete RS cycle using

(a) $3\text{ V} \rightarrow -2\text{ V} \rightarrow 3\text{ V}$ with a period of 10 ms triangular wave bias signal and (b) $3/-2\text{ V}$ with a period of 10 ms rectangular wave bias signal [37].

and using the same initial state (LRS). The simulated $R-t$ behaviour for $D = 4\text{ nm}$ device using triangular and rectangular input signals are shown in Figure 5.9(a) and (b), respectively. The input signals are also shown in Figure 5.9. The applied triangular signal has a sweeping sequence of $3\text{ V} \rightarrow -2\text{ V} \rightarrow 3\text{ V}$ with a period of 10 ms. It can be seen in figure Figure 5.9(a) that when the voltage sweeps from $0\text{ V} \rightarrow 3\text{ V}$, the device resistance is initially at LRS ($30\text{ k}\Omega$). Once the sweeping voltage reaches HSV (1.9 V), the resistance increases gradually into its HRS value ($151.5\text{ k}\Omega$). However, during the voltage sweeping from 3 V to -2 V and before LSV is reached, the same behaviour when a sinusoidal signal was used is observed again where the device maintains its HRS until the voltage becomes negative and then the device shows the same temporal increase in its HRS with the same resistance of around $4.8\text{ M}\Omega$. Once LSV is reached, the resistance switches abruptly to its LRS value ($30\text{ k}\Omega$). Figure 5.9(b) shows similar behaviour and the same values of LRS and HRS obtained when a rectangular input signal is used.

The results in Figure 5.9 indicate that the device can fully switch between the same values of HRS and LRS and also showing the same values of HSV and LSV despite the type of the input signal. Accordingly, this SPICE model provides a highly accurate and predictive $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM model that can be used for the future memory applications, especially logic design circuits based on pulse signals. This is considered as a major advantage when compared to the other bi-layered models which have not been tested under the same input signals.

To further verify the validity of the proposed model, we conduct pulse switching simulation with different RESET pulse amplitudes. Comparison between the model simulation and the experimental results from [17] are shown in Figure 5.10(a). The simulated and the experimental



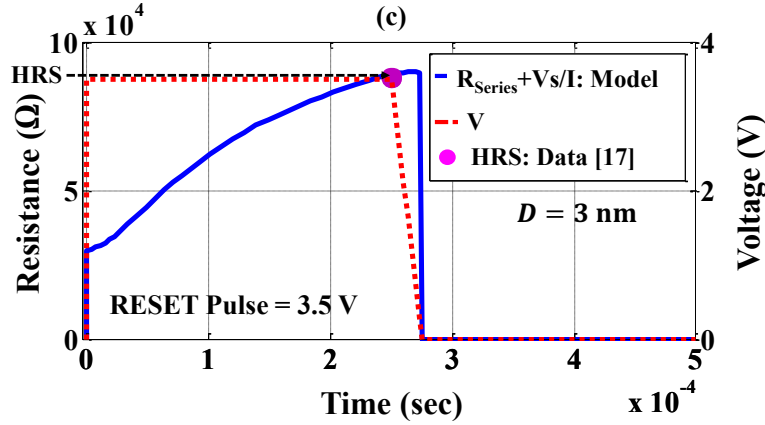


Figure 5.10. (a) Experimental measurements of the Ta₂O₅/TaO_x bi-layered RRAM [17] and simulation results of the proposed SPICE model for RESET pulse switching operation with $D = 3$ nm, $\Phi_{Bn0} = 0.45$ eV, $\xi = 0.0031$ eV, $R_{OFF} = 20$ k Ω , $x_1 = 95$, $x_2 = 0.03$, $n_1 = 0.1905$ (b) Time domain response simulation of the current compared with the measured current at HRS (I_{HRS}) (c) Time domain response simulation of the resistance compared with the experimental resistance at HRS. The simulation results in (b) and (c) are obtained by applying a single RESET pulses of 3.5 V, similar to (a) [37].

data are obtained using the same bias protocol of a RESET pulse voltage of 500 ns duration time with an initial RESET amplitude of 3.5 V which increases by 0.5 V for every 250 μ s [17].

It can be seen that the model can successfully demonstrate the current change with regards to RESET pulse voltages. The model simulation results match with the measured data with excellent agreements. Figure 5.10(b) and (c) show the time domain response simulation of the current and resistance obtained by applying one of the single RESET pulses (3.5 V) used in the experiment in Figure 5.10(a) with the same width. Also shown the measured current at HRS (I_{HRS}) and the experimental resistance at HRS, both obtained at the end of a RESET pulse signal of 3.5 V [extracted from Figure 5.10(a)]. The SPICE model accurately reproduced the same I_{HRS} and the resistance value at HRS and showed very good coincidence with their corresponding experimental values which further justify the validation of the model. It can be seen in Figure 5.10(b) that when a single pulse of RESET transition is applied, the response current is increased, following the voltage increment (because the initial device state is LRS)

and the same behaviour was reported in [18]. Figure 5.10(b) also shows that the model can predicts the gradual RESET transition behaviour as reported in [17] and [21].

5.3.6. RRAM-Based Non-Volatile D-Latch

As an application of the proposed $\text{Ta}_2\text{O}_5/\text{TaO}_x$ RRAM SPICE model, a RRAM-based NV D-latch circuit is designed. Figure 5.11 shows the NV D-latch circuit design where the proposed RRAM model acts as a NV element that retains the latched data in the event of the power interruption. The SPICE simulation results of the NV behaviour of the D-latch is illustrated in Figure 5.12(a).

It can be seen in Figure 5.12(a) that between $t = 0$ to 0.1 ms, G is at low (\bar{G} is high) and the input data D_{in} is kept at high. Therefore, the transmission gate TG1 is turned-off and TG2 is turned-on. The data in the latch during this period is invalid or depends on the previous state of the latch. During $t = 0.1$ – 0.3 ms, G is high and that turns-on TG1 and turns-off TG2. Now, the data D is written into the back-to-back connected inverter. Hence, D is high and \bar{D} is low.

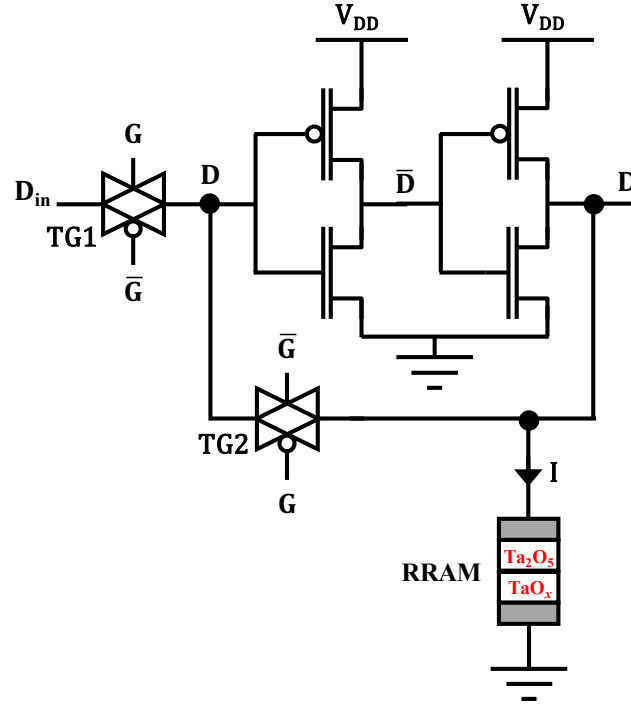


Figure 5.11. Schematic of the RRAM-based NV D-Latch with the Ta₂O₅/TaO_x RRAM SPICE model integrated [37].

At the same duration, the data is also written into the RRAM. It can be observed from the simulation results in Figure 5.12(a) that the current I flowing through the RRAM decreases from 80 μA (at 0.1 ms) to 18 μA (at 0.3 ms) and this is due to the resistance of the RRAM which is initially at LRS and then changes to HRS. At $t = 0.3$ ms, G goes to low, hence, TG2 is turned-on and TG1 is turned-off. This retains the data in the latch and the HRS in the RRAM. When a power interruption occurs at $t = 0.4$ ms ($V_{DD} = 0$ V), it can be observed that D , \bar{D} , and the current through the RRAM are low. Then at $t = 0.42$ ms, when the power resumes ($V_{DD} = 3$ V), the current through the high resistance RRAM (18 μA), retains the original value of D (to high) and \bar{D} (to low). Thus, the data is successfully retained in the latch.

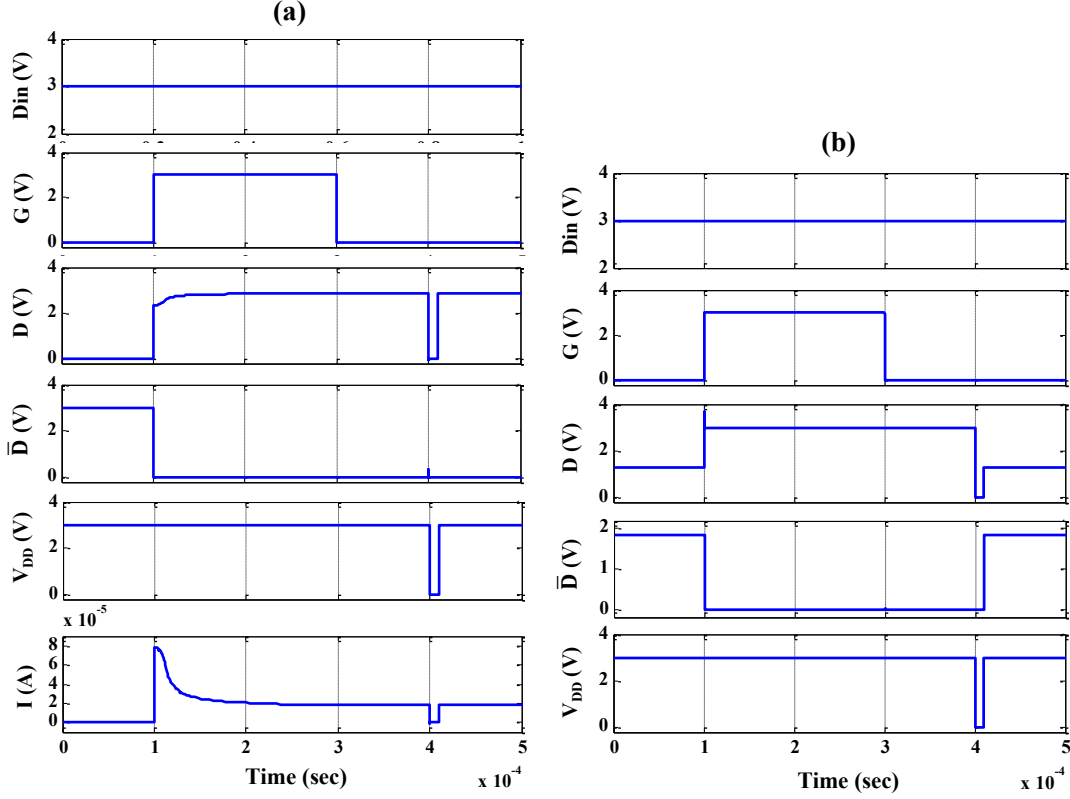


Figure 5.12. The SPICE simulation of the RRAM-based NV D-Latch (a) with the Ta_2O_5/TaO_x RRAM SPICE model integrated and (b) without the RRAM connected [37].

Next, RRAM is removed from the D-latch circuit and the simulation is performed on the circuit under the similar simulation environment setup of the NV D-latch. The simulation results without the RRAM connected are shown in Figure 5.12(b). It can be observed from the results that at $t=0.42$ ms, when the power resumes, D and \bar{D} do not resume to their original states after the power interruption and hence, the latched data is corrupted. Thus, an application of the proposed Ta_2O_5/TaO_x RRAM SPICE model as a non-volatile element in the RRAM-based NV D-latch is demonstrated successfully.

5.3.7. Computational Efficiency

An efficient SPICE model for the bi-layered RRAM device should successfully reproduce the device response to the applied switching bias and maintain the computational efficiency at the same time. It is expected that the physics-based approach used in the proposed model provides an enhanced accuracy at the expense of a longer computational time. The simulation engine that is used to run the SPICE model can also affect the computational time. Therefore, to improve the computational efficiency of the proposed SPICE model, the static and the dynamic equations in the LTSPICE sub circuit implementation in Figure 5.3 are separated into simpler equations and implemented using the inbuilt circuit components such as VCCS (G-type source in LTSPICE) and VCVS (E-type source in LTSPICE). Finally, during the simulation of our model, the timestep parameter provided a trade-off between the model accuracy and the computational time where increasing the computational efficiency (by increasing the timestep) resulted in convergence problem.

5.3.8. Testing the Applicability of the Proposed Model for simulation of RS Behaviour

Besides the verifications with three different sets of experimental data, successfully testing the model under pulse switching operation with different RESET pulse amplitudes, and integrating the model in a RRAM-based circuit application, the proposed SPICE model is also analysed under one of the evaluation criteria reported in [44]. The model is checked to verify its ability to reproduce some distinct features of the basic bipolar resistive switching I – V behaviour of

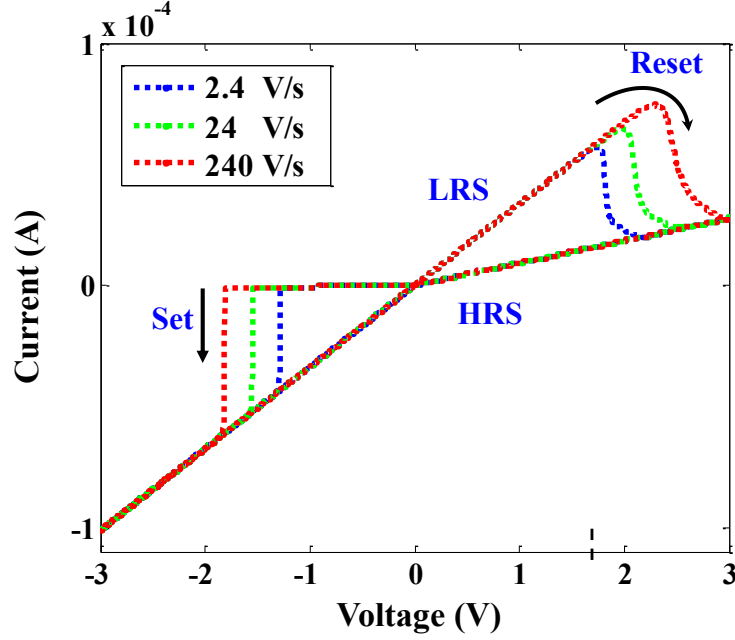


Figure 5.13. Sweep rate dependency of the I - V characteristic of the proposed SPICE model. The simulated I - V characteristic are obtained by applying symmetric sinusoidal signals of three different voltage sweep rates: 2.4 V/s, 24 V/s, and 240 V/s [37].

the physical MISM RRAM device (first criteria in [44]). However, in the future, we also consider testing the model for the presence of sufficient nonlinearity of the switching kinetics (second criteria in [44]) and integrating the model in a multi-element simulation (e.g. two element circuit in a complementary resistive switch) which is the third criteria in [44]. This is considered as a further verification of the validity of the proposed model when integrated in a circuit application.

First Criteria in [44]: The physical MISM RRAM studied in this research is based on the valence change mechanism (VCM) [44]. Hence, an abrupt SET and gradual RESET are expected for its resistive switching [21], [44]. It can be seen in the simulation results in figures Figure 5.4–Figure 5.6 that the proposed model can capture the abrupt and the gradual SET and RESET respectively, with a very good matching with the measured data. Furthermore, the I - V

characteristics of the physical MISM RRAM are asymmetric with respect to the origin which can also be successfully reproduced by the proposed model (See figures Figure 5.4–Figure 5.6). The model can also demonstrate the general trend of a higher SET and RESET voltages for increasing voltage sweep rate as reported in [44]. Figure 5.13 shows the simulation results achieved by applying three symmetric sinusoidal signals with different sweep rates of 2.4, 24, and 240 V/s. The obtained simulation results show that the model depicts higher SET and RESET voltage for increasing sweep rate, in agreement with the previous results of VCM [44].

A PREDICTIVE COMPACT SPICE MODEL OF TaO_x-BASED MIM RRAM

Summary

Among the available RS materials, Tantalum oxide demonstrated encouraging RS behaviour and properties. As mentioned in this thesis report, this material showed favourable endurance, RS speed, multilevel property, and stable phases. However, in order to have a complete library for a Tantalum-oxide-based RRAM SPICE models, an MIM RRAM SPICE model is also required besides the MISM RRAM model developed in chapter 5. In this chapter, a predictive compact MIM SPICE model for RS in Tantalum-oxide-based RRAM is developed. The proposed compact model is developed based on the analytical predictive MIM model of Pt/TaO_x/Ta RRAM in [42] which is compatible with SPICE. Although this model is not based on all the physics involved in the device RS and current conduction mechanisms (like the bilayered RRAM model developed in this thesis report), it is considered an important first step toward understanding the physical insight behind these mechanisms.

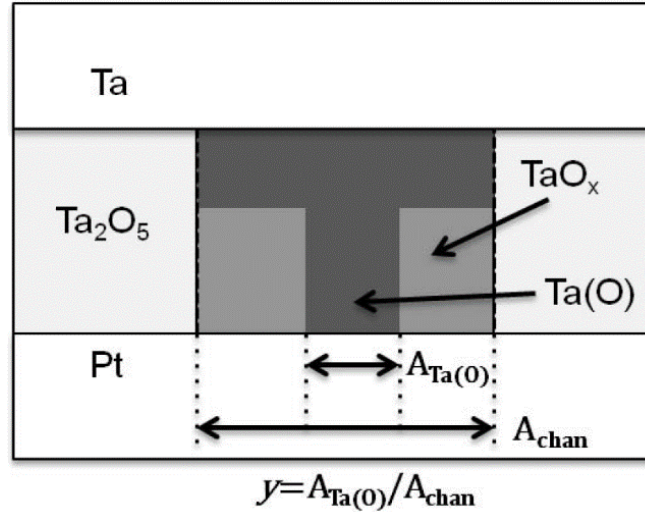


Figure 6.1. Schematic representation of the Ta/TaO_x/Pt MIM RRAM cell modelled in this chapter showing the pattern of the oxygen depletion region in this device and the state variable y [42].

6.1. The Structure and the RS Mechanism of the Proposed MIM SPICE Model

The MIM RRAM model in [42] provides an analytical approximation of Leon Chua memristor static and dynamic equations for the Ta/TaO_x/Pt RRAM. This model is strongly grounded in experimental data and developed after studying the electronic transport and the RS dynamics in Ta/TaO_x/Pt MIM RRAM. The structure of the oxide-based Ta/TaO_x/Pt RRAM cell modelled in this chapter is shown in Figure 6.1, which consists of a thin amorphous layer of Ta₂O_{5-x}, sandwiched between two metal electrodes of Ta (TE) and Pt (BE). The thickness of the Ta₂O_{5-x} layer is 4–10 nm.

In this MIM RRAM, the transport in the ON state is dominated by a subregion (or a channel) of the RRAM device [42] (see Figure 6.1). The region around and within this conducting channel indicates modification of the original ratio of Ta:O where O is partially depleted in this channel and the concentration of O increases outside the active channel. The structure around

the channel is modified where the phase of the initially deposited amorphous film is changed into a nanocrystalline phase. This behaviour indicates local heating. The schematic representation of this pattern and the oxygen depleted regions are shown in Figure 6.1 [42].

In the extreme ON and OFF cases, the full film thickness is Ta_2O_5 and Ta with dissolved O [Ta(O)], for the OFF (insulating channel) and ON (metallic channel) states, respectively [42]. These are the two thermodynamically two stable phases of the Ta-O system.

6.2. Modelling of the Dynamic Behavior – SET and RESET Processes

According to [42] and from the explanation in the previous section, the Ta/TaO_x/Pt MIM RRAM state variable describes the oxygen contents in the conducting channel shown in Figure 6.1. Therefore, the state variable in this model reflects a changing ration of the two parallel phases: Ta_2O_5 and Ta(O), each with different oxygen compositions. In this chapter, the state variable will be denoted y (see Figure 6.1), which will reflect the cross-sectional area (or the volume fraction) of the Ohmic region (metallic region) in the channel. The remaining fraction of the channel ($1-y$) is assumed insulator. These two volume fractions have linear and nonlinear $I-V$ dependence for metallic and insulator regions, respectively [42]. The state variable y in this model is given by the ratio:

$$y = A_{\text{Ta(O)}}/A_{\text{Channel}} \quad (1)$$

where $A_{\text{Ta(O)}}$ and A_{Channel} are the cross sectional areas of the metallic channel and the total channel area while in the insulating state, respectively [42].

The RESET switching in this MIM RRAM is obtained by applying negative bias on TE. The RESET switching dynamics showed best fitting when an exponential voltage-controlled switching behaviour is used. It also showed additional dependence on the power (Joule heating effect) which slow down the RESET process. The RESET switching dynamic model used in [42] is given by equation (2) which showed best fitting to the experimental data.

$$\frac{dy}{dt} = A \cdot \sinh \left[\frac{V}{\sigma_{\text{OFF}}} \right] \cdot \exp \left[- \left(\frac{y_{\text{OFF}}}{y} \right)^2 \right] \cdot \exp [1/(1 + (1 + \beta p))] \quad (V < 0) \quad (2)$$

where A , σ_{OFF} , y_{OFF} , and β are fitting parameters. The value of these parameters are provided in Table 6-1. p is the power which shows that Joule heating slow down RESET process. The SET switching dynamics of the Ta/TaO_x/Pt MIM RRAM in [42] is given by the following equation [42]:

$$\frac{dy}{dt} = B \cdot \sinh \left[\frac{V}{\sigma_{\text{ON}}} \right] \cdot \exp \left[- \left(\frac{y}{y_{\text{ON}}} \right)^2 \right] \cdot \exp [p/\sigma_p] \quad (V < 0) \quad (3)$$

where B , σ_{ON} , y_{ON} , and σ_p are fitting parameters.

The value of these parameters are provided in Table 6-1. It can be seen that the SET process has opposite dependence on the power p when compared to the RESET process where Joule heating speeds up the SET process. Although this equation showed good agreement with the experimental data when the applied voltage is above the threshold voltage, it resulted in inadequate results at the near-threshold voltage (around 0.5 V) [42].

By comparing equations (2) and (3), it can be seen that the SET and RESET switching dynamics have the same form of voltage dependence [42]. Both have an exponential dependence on the applied voltage where a very small increase in the applied voltage results in

orders of magnitude faster switching process, which is in agreement with the characteristics of the Tantalum-Oxide RRAM [42].

6.3. Modelling of the Static Behavior – Current Conduction Process

According to [42], the conduction during LRS for this MIM RRAM model is metallic whereas the conduction during HRS showed good fitting using the nonlinear Frenkel-Poole equation [42]. The conduction equation of the device in Figure 6.1 is giving be the following equation [42]:

$$I = V [yG_m + (1 - y)a \cdot \exp(b\sqrt{|V|})] \quad (4)$$

where I is the current through the device, V is the total voltage across the RRAM device, a , b , and G_m are constants depends on the material of the conduction channel and can be used a fitting parameters in the SPICE model. These constants are fixed for a particular cell despite of its state.

The expression $[yG_m + (1 - y)a \cdot \exp(b\sqrt{|v|})]$ represents the parallel combination of the two phases shown in Figure 6.1. When a positive voltage is applied on TE (SET switching), the linear metallic phase Ta(O) fills the channel ($A_{\text{Ta(O)}} = A_{\text{Channel}}$) and the state variable y reaches 1. Hence, from equation (4), the conductance of the RRAM become G_m . Conversely, when a negative voltage is applied on TE (RESET process), the device reaches its HRS when the insulating oxide fills the entire channel ($A_{\text{Ta(O)}} = 0$) and state variable y become 0. As a results, the conductance in equation (4) become $a \cdot \exp(b\sqrt{|v|})$ which describes the nonlinear

Frenkel-Poole transport mechanism. Similar to the bi-layered RRAM SPICE model developed in this research, it can be seen in equation (4) that the current conduction model in [42] does not take into consideration Joule heating effect.

The power in equations (2) and (3) (which reflects Joule heating effect) is given by the multiplication of the total voltage across the RRAM device and the current passing through the RRAM as follows:

$$P = V \cdot I \quad (5)$$

6.4. SPICE Model Implementation

The mechanisms of y evolution and the current conduction are summarized in the related equations (1)–(5) and have been implemented in LTSPICE as a single Ta/TaO_x/Pt device. Table 6-1 includes the parameters used in SPICE simulation with their values. The structure of the SPICE model is shown in Figure 6.2 which determines the single device time-dependent current flow at LRS, HRS and the transitional state. The equivalent SPICE subcircuit implementation of this structure is shown in the listing in Figure 6.3.

It can be seen in Figure 6.2(a) and the listing in Figure 6.3 that the single Ta/TaO_x/Pt RRAM device is represented by the two terminals SPICE subcircuit where TE and BE in Figure 6.2(a) corresponds to plus and minus in Code line 02 in Figure 6.3. The current port equation of the subcircuit is composed of two elements in parallel connection as shown in the top part of Figure 6.2(a) (code lines 09–15). These two elements are VCCS, GLinear and GNonLinear (G-type source in LTSPICE) which model the linear $[yG_m]$ and the nonlinear $[(1 - y)a \cdot \exp(b\sqrt{|V|})]$

Table 6-1. Parameters Used in the proposed MIM SPICE RRAM model simulation.

Parameter	VALUE	SPICE Model Symbol
G_m	0.02	Gm
a	7.5e-6	a
b	4.7	b
A	8e-11	AOFF
σ_{OFF}	0.0155	SegOFF
y_{OFF}	0.05	yOff
β	500	Bita
B	4	BON
σ_{ON}	0.35	SegON
y_{ON}	0.042	yON
σ_p	2.65e-5	Segp

current behaviour, respectively. The current I passing through this circuit is the total current through the MIM RRAM device as given by (4). The terminal voltages of the VCVSs: Es1, Es2, and Es3 represent the detailed implementation of GLinear and GNonLinear based on equation (4).

In the second part of the SPICE listing, code lines 16–25 depict the implementation of the circuit structure in Figure 6.2(b) which includes the modelling of y evolution dynamic. In line 17, a VCVS Epw is used to represents the implementation of the power (due to Joule heating effect). Two VCCSs, GON and GOFF are used to produce the current $I_y = \frac{dy}{dt}$ using (2) and (3), respectively [see Figure 6.2(b)]. Based on the applied bias polarity, the function STP is used to switch-on GON ($I_w = GON$) when $V > 0$ (switching into LRS) while GOFF is used ($I_w = GOFF$) when $V < 0$ (switching into HRS). The instantaneous value of y is achieved by integrating the current I_y in Figure 6.2(b). The integration is performed by taking the voltage $V(dy/dt)$ across the capacitor C_y [see Figure 6.2(b)]. The capacitor C_y has a value of 1 F in

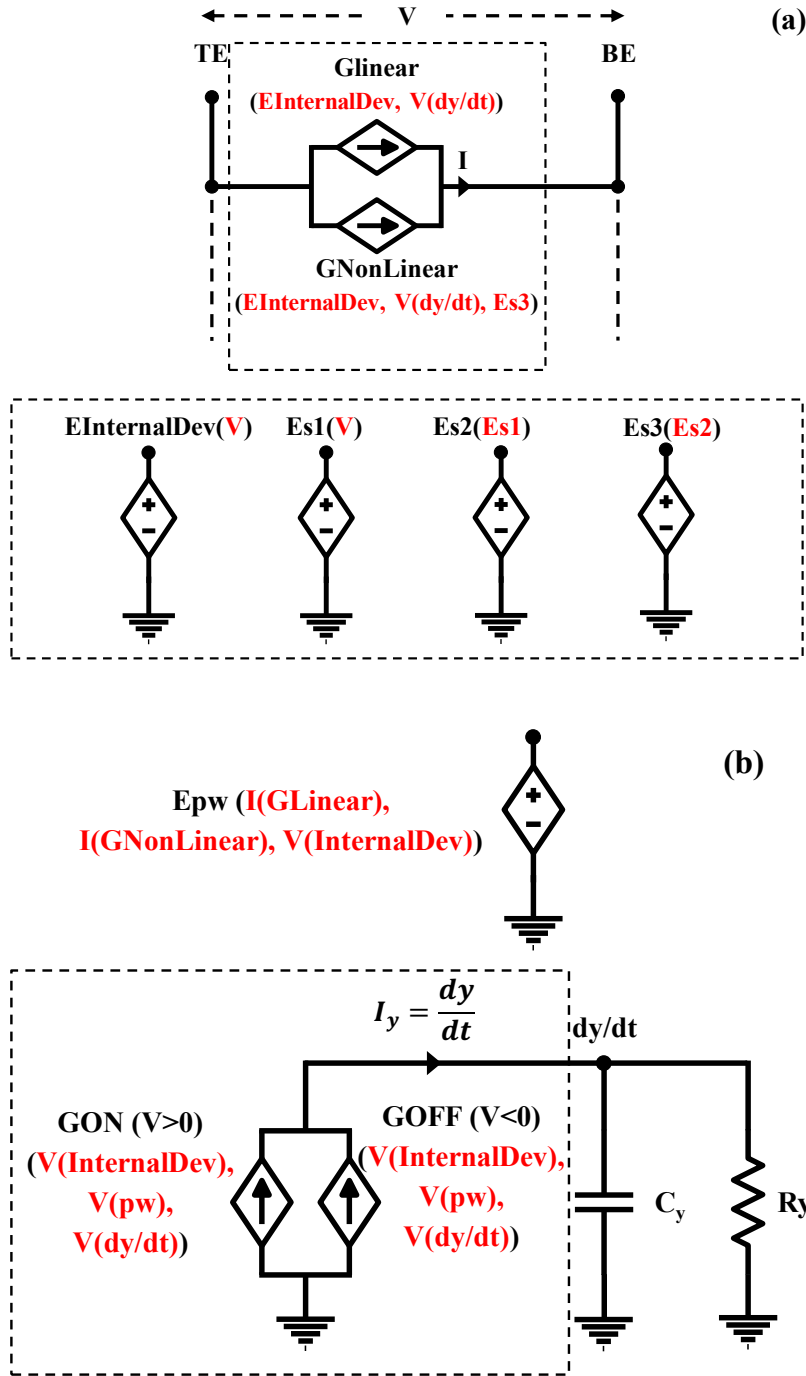


Figure 6.2. LTSPICE implementation of the proposed MIM SPICE model. (a) The two terminal (current path) SPICE implementation of the single Ta/TaO_x/Pt device and the implementation of the related parameters. (b) The SPICE subcircuit implementation of y evolution.

```

01 *Ta/TaOx/Pt MIM RRAM
02 .SUBCKT TaOxRRAM plus minus PARAMS:
03 *Static Model Parameters
04 + Gm=0.02 a=7.5e-6 b=4.7
05 *Dynamic Model Parameters for ON Switching
06 + BON=4 SegON=0.35 yON=0.042 Segp=2.65e-5
07 *Dynamic Model Parameters for OFF Switching
08 + AOFF=8e-11 SegOFF=0.0155 yOff=0.05 Bita=500
09* Static Behaviour Modelling of the MIM RRAM
10 ElInternalDev InternalDev 0 value={V(plus,minus)}
11 Es1 s1 0 value={abs(V(InternalDev))}
12 Es2 s2 0 value={exp(b*sqrt(V(s1)))}
13 Es3 s3 0 value={a*V(s2)}
14 GLinear plus minus value={V(InternalDev)*(V(y)*Gm)}
15 GNonLinear plus minus value={V(InternalDev)*((1-V(y))*V(s3))}
16 * Dynamic Behaviour Modelling of the MIM RRAM
17 Epw pw 0 value={((GLinear)+I(GNonLinear))*V(InternalDev)}
18 *Dynamic ON switching (V>0)
19 GON 0 y value={{BON*sinh(stp(V(InternalDev))*V(InternalDev)/SegON)*exp(-
20 +((V(y)/yON)**2))*exp(V(pw)/Segp)}}
21 *Dynamic OFF switching (V<0)
22 GOFF 0 y value={{AOFF*sinh(stp(-V(InternalDev))*V(InternalDev)/SegOFF)*exp(-
23 +((yOFF/V(y))**2))*exp(1/(1+(Bita*V(pw))))}}
24 Cy y 0 1 IC=0.007
25 Ry y 0 1T
26 .ENDS TaOxRRAM

```

Figure 6.3. LTSPICE subcircuit implementation of the proposed MIM SPICE model.

order to keep the units of y unchanged. Furthermore, in order for the simulation to determine the initial DC operating point, a dc path from point dy/dt to the ground is provided using a resistor R_y with a very large value as in code line 25.

6.5. Model Evaluation and Simulation Studies

The MIM RRAM equations provided in sections 6.2 and 6.3 have been evaluated by simulation using LTSPICE. The simulation was done using the same effective circuit used in the experimental measurements and the simulation in [42]. This circuit uses an external resistance

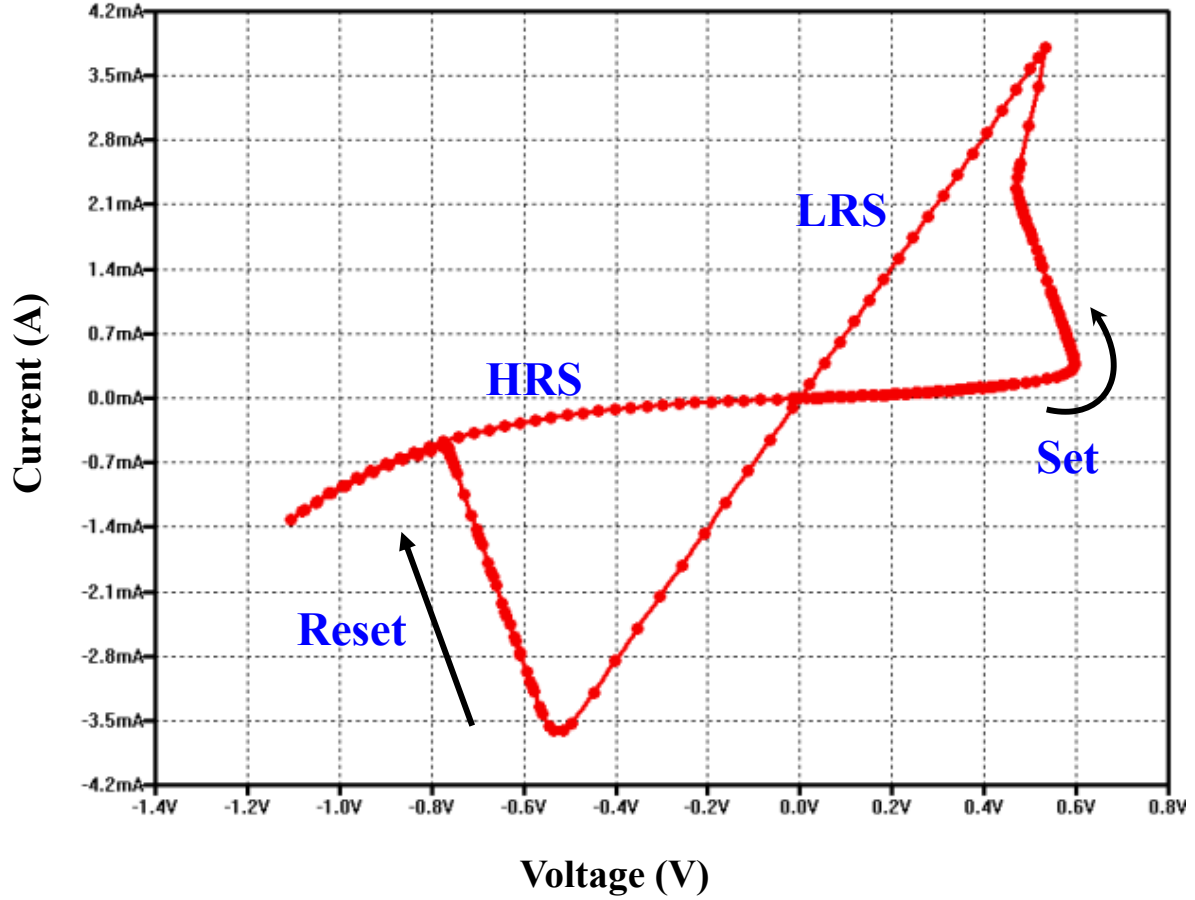


Figure 6.4. The linear scale plot of the MIM SPICE model simulation I - V characteristics with a voltage sequence of sawtooth signal 0, 0.8, 0, -1.2, and 0 V and sweep time of $1e-4$ s.

R_{ext} connected in series with the MIM RRAM and the voltage source. The total external resistance R_{ext} is the resistance of the source impedance, the device electrodes, and the input impedance of the measurement unit. The values of these resistances depend on the time scale probed and the RRAM electrodes width and thickness [42]. The external resistance is considered in [42] because the RRAM LRS resistance value is comparable to the external resistance used in the measurements in [42]. Hence, the voltage divider effect becomes important. However, in the bi-layered RRAM modelled in this report, the external resistance

of the circuit containing the RRAM device is assumed to be neglected during the experimental measurement which is why it was not considered in the proposed model in chapters 4 and 5.

Figure 6.4 show the simulation results of the proposed MIM SPICE model obtained using sawtooth voltage cycle. The voltage sequence of the sawtooth signal is 0, 0.8, 0, -1.2, and 0 V and the sweep time is $1e^{-4}$ s [42]. The value of R_{ext} is $70\ \Omega$. The proposed model is correlated against several published characteristics of the Ta//TaO_x/Pt RRAM and a number of different insights and matched features emerged. Similar to the simulation results of the analytical MIM RRAM model obtained in [42], the simulation results in Figure 6.4 show that the device is switching to LRS and HRS by positive and negative voltage, respectively. Also, the nonlinearity of the dynamics can be easily observed by abrupt increase and decrease in the device current as the applied bias reach its positive and negative switching voltages, respectively, which is in agreement with the characteristic of the MIM RRAM device reported in [42]. The model also reproduced well most of the $I-V$ characteristics reported in the experiments in [42]. However, this model is still under developments and more physics-based insights will be added to the model in the future in order to increase its accuracy and the reproducibility of the experimental results of the Ta/TaO_x/Pt MIM RRAM devices.

CONCLUSION AND FUTURE WORK

In this research, a physics-based mathematical and SPICE models for the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM have been developed. A new term TPF which manifests the dependency of the $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM current on the physical characteristics of the insulator layer is used. The proposed models emphasize the effect of the continuous variation of the interface traps density and the ideality factor on the current conduction. In addition, the oxygen ion migration mechanism is predicted by deriving the electric field equation for the active region in the MISM structure. Moreover, the self-limiting growth of the doped region has also been demonstrated.

The proposed SPICE model offers different adjustable parameters which make it easy to fit the model into different $\text{Ta}_2\text{O}_5/\text{TaO}_x$ bi-layered RRAM devices with switching layer thickness smaller than 5 nm (3 and 4 nm). The SPICE model has successfully reproduced all the main aspects from experimental results for the SET and RESET processes and also the asymmetric and the symmetric current profiles in HRS and LRS, respectively. The SPICE model can also demonstrate the current change with regards to RESET pulse signal of different amplitudes. The developed SPICE model has showed a stable behaviour for its HRS and LRS regions under three different types of the conventional voltage input signals. Finally, an application of the

proposed Ta₂O₅/TaO_x bi-layered RRAM SPICE model as a non-volatile element in the RRAM-based NV D-latch is demonstrated successfully.

Future work would include more effort on enhancing the proposed models behaviour in HRS region by taking OCF region into account when designing the model. In addition, future work involves investigating the possibility to extend the model to represent Ta₂O₅/TaO_x bi-layered RRAM devices with thicker switching layers and also other bi-layered RRAM physical devices based on different oxide material. This can be done by verifying the structural models of bi-layered RRAM devices of different materials using device simulator (e.g. Synopsys TCAD). It also includes studying the temperature dependence, the statistical variability, and the noise characteristics of the Ta₂O₅/TaO_x bi-layered RRAM devices.

The future work also considers testing the models for the presence of sufficient nonlinearity of the switching kinetics (second criteria in [44]) and integrating the model in a multi-element simulation (e.g. two element circuit in a complementary resistive switch) which is the third criteria in [44]. This is considered as a further verification of the validity of the proposed models when integrated in a RRAM-based circuit application.

Future work would also include developing a Verilog-A model of the Ta₂O₅/TaO_x bi-layered RRAM which can also be used in SPICE-based circuit simulations.

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9. Appendix A

MATLAB SCRIPTS AND LTSPICE SUBCIRCUITS

9.1. MATLAB Scripts for the Proposed MISM Mathematical RRAM Model Presented in Chapter Four

9.1.1. MATLAB Script for $D = 4$ nm

```
clear all, close all, clc
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Constants
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
To= 300; % Room Temperature
D = 4e-9; % Ta2O5 Thickness
Vt = 0.02585; % Thermal Voltage VT = KT/q.
Aa = 9e-10; % Electrode area
eo = 8.85418782e-12; % free space permittivity value
K=1.3806e-23;
e=1.60217646*10^(-19); % Electron Charge
KT = 0.026; % in eV
As = 120e4;
N = 1e23; % Constant
es = 27*eo; % Ta2O5 permittivity value
Phi_T = 0.00175; % (In eV) Constant
Roff =4e4; % Resistance of Fully Undoped state
Ron = 1700; % Resistance of fully doped state change
Ro =12000; % Bulk Layer Resistance
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Time Axis & Applied External Voltage
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
num_of_cycles = 1
freq = 100; %Applied bias signal frequenvy
```

```

tspan=[0 num_of_cycles/freq];
points=2e4;
tspan_vector = linspace(tspan(1),tspan(2),points);
amp =2; % Applied bias voltage amplitude
V=zeros(size((tspan_vector)));
V = amp*sin(freq*2*pi*tspan_vector); %The applied external voltage
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%RRAM Initial Values - Initial State
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
W=zeros(size((tspan_vector)));
W_dot=zeros(size((tspan_vector)));
D_Phi=zeros(size((tspan_vector)));
Phi_s=zeros(size((tspan_vector)));
Eta=zeros(size((tspan_vector)));
Phi_B = zeros(size((tspan_vector)));
Phi_Bo = zeros(size((tspan_vector)));
Is= zeros(size((tspan_vector)));
E= zeros(size((tspan_vector)));
Vsch=zeros(size((tspan_vector)));
VD=zeros(size((tspan_vector)));
T=zeros(size((tspan_vector)));
R=zeros(size((tspan_vector)));

% The initial state of the RRAM is the fully doped state w=0 (LRS)
w_init = 0.0;
W0=w_init*D;
delta_t=tspan_vector(2)-tspan_vector(1);
W(1)=W0;
R(1) = Ron+Ro;
Itun(1) = V(1)/R(1);
T(1)=300;
Vsch(1)=(V(1)-(Itun(1).*R(1)));
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Schottky Barrier and tunneling equations
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
f=1e13;
a=1e-9;
U=1;
Rth=1e8;

for i=2:length(tspan_vector)

Phi_Bo(i-1)=0.6.*((W(i-1)./D));
D_Phi(i-1) = (((e^3).*N.*Phi_Bo(i-1))/((8.*(pi^2)).*es^3)).^0.25);
Phi_B(i-1) = Phi_Bo(i-1) - D_Phi(i-1);
R(i-1)=(Ro+(Ron*(D-W(i-1))/D)+(Roff*W(i-1)/D));
Eta(i-1)=60000*((1000*(D-W(i-1))/D)+(900*W(i-1)/D));
    if V(i-1) < 0

```

```

        Is(i-1)=Aa*As*(To^2)*exp(-Phi_B(i-1)/(5.35*K*To/e));
        Itun(i)=Is(i-1).*(exp(Vsch(i-1)/(Eta(i-1).*Vt))-1).*exp(-W(i-
1)*1e10*sqrt(Phi_T));
        elseif V(i-1) >= 0
            Is(i-1)=Aa*As*(To^2)*exp(-Phi_B(i-1)/(85*K*To/e));
            Itun(i)=-Is(i-1).*(exp(-Vsch(i-1)/(Eta(i-1).*Vt))-1).*exp(-W(i-
1)*1e10*sqrt(Phi_T));
            end;

if V(i) <= 0
Vsch(i)=(V(i)-(Itun(i).*R(i-1)));
VD(i)=(V(i)-(Itun(i).*Ro)-Vsch(i));
E(i)=VD(i)/(W(i-1)+((Ron/Roff)*(D-W(i-1))));
T(i)=To+(Rth*(Itun(i)^2*(R(i-1)-Ro)));
W_dot(i)=a*f.*exp(-U*e/(K*T(i))).*sinh((163*e*a*E(i))/(1*K*T(i)));
elseif V(i)>0
V(i) = 3*sin(freq*2*pi*tspan_vector(i));
Vsch(i)=(V(i)-(Itun(i).*R(i-1)));
VD(i)=(V(i)-(Itun(i).*Ro)-Vsch(i));
E(i)=VD(i)/(W(i-1)+((Ron/Roff)*(D-W(i-1))));
T(i)=To+(Rth*(Itun(i)^2*(R(i-1)-Ro)));
W_dot(i)=.6e-6*a*f.*exp(-U*e/(K*T(i))).*sinh((.4*e*a*E(i))/(1*K*T(i)));
end;
W(i)=W(i-1)+W_dot(i)*delta_t;

if W(i) <= 0
    W(i) = 0;
    W_dot(i)=0;
elseif W(i) > D
    W(i) = D;
    W_dot(i)=D;
end

end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Simulation Plots
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
subplot(2,4,1)
plot(tspan_vector,W/D,'r');

subplot(2,4,2)
plot(tspan_vector,V);
title('V-t curve');
xlabel('T[Sec]');
ylabel('V[Volts]');

subplot(2,4,3)
plot(W/D,E);
title('V-E curve');
xlabel('W/D');
ylabel('E (V/m)');

```

```

subplot(2,4,4)
plot(tspan_vector,Itun);
title('I-t curve');
xlabel('T[Sec]');
ylabel('I[Amps]');

subplot(2,4,5)
plot(V,Itun);
title('It-V1 Linear curve');
xlabel('V1[volt]');
ylabel('It[amp]');

subplot(2,4,6)
plot(tspan_vector,Vsch)
title('Vsch');
xlabel('T[Sec]');
ylabel('Vsch[volt]');

subplot(2,4,7)
plot(V,R);
% title('');
xlabel('Voltage(V)');
ylabel('Resistance(?)');

subplot(2,4,8)
plot(V, Phi_B);
xlabel('Voltage(V)');
ylabel('Phi_b[eV]');

%Matlab model Results - I-V
data=xlsread('D4nm_ExpData.xlsx');
xAxis=data(:,1);
yAxis=data(:,2);
figure(2);
semilogy(V,abs(Itun));
hold;
semilogy(xAxis,abs(yAxis));
xlabel('Voltage (V)');
ylabel('Current (V)');

% SPICE model Results - Semilog I-V
data1=xlsread('SPICE_D4nm.xlsx');
xAxis1=data1(:,1);
yAxis1=data1(:,2);
xAxis2=data1(:,3);
yAxis2=data1(:,4);
figure(3);
semilogy(xAxis1,abs(yAxis1));
hold;
semilogy(xAxis2,abs(yAxis2));
% plot(xAxis1,yAxis1,xAxis2,yAxis2);
xlabel('Bias Voltage (V)');
ylabel('Current (A)');

%SPICE model Results - Linear I-V
data1=xlsread('SPICE_D4nm_ForLinearIV.xlsx');

```

```

xAxis1=data1(:,1);
yAxis1=data1(:,2);
xAxis2=data1(:,3);
yAxis2=data1(:,4);
figure(4);
plot(xAxis1,(yAxis1));
hold;
plot(xAxis2,(yAxis2));
xlabel('Bias Voltage (V)');
ylabel('Current (A)');

figure(5);
semilogy(V,abs(E));
xlabel('Voltage (V)');
ylabel('E (V/m)');

figure(6);
plot(tspan_vector,VD,'g');
hold;
plot(tspan_vector,Itun*Ro,'b',tspan_vector,Vsch,'r');
title('VD-Itun*Ro-Vsch');
xlabel('T[Sec]');
ylabel('V[volt]');

figure(7);
plotyy(tspan_vector,VD,tspan_vector,R-Ro,'plot','plot');
xlabel('T[Sec]');
ylabel('Ri');

%SPICE model Results - The temporal increase in HRS
data2=xlsread('Temp_Incr_HRS.xlsx');
yAxis01=data2(:,1);
yAxis02=data2(:,2);
yAxis03=data2(:,3);
yAxis04=data2(:,4);
yAxis05=data2(:,5);
yAxis06=data2(:,6);
yAxis07=data2(:,7);
yAxis08=data2(:,8);
figure(8);
plot(yAxis01,yAxis02,'g');
hold;
plot(yAxis01,yAxis03,'b',yAxis01,yAxis04,yAxis01,yAxis05);
figure(9);
plotyy(yAxis01,yAxis07,yAxis01,yAxis08,'plot','plot');

%SPICE model Results - Triangular
data3=xlsread('Tria_Input.xlsx');
yAxis001=data3(:,1);
yAxis002=data3(:,2);
yAxis003=data3(:,3);
figure(10);
plotyy(yAxis001,yAxis003,yAxis001,yAxis002,'plot','plot');

%SPICE model Results - Rectangular

```



```

data4=xlsread('Rect_Input.xlsx');
yAxis0001=data4(:,1);
yAxis0002=data4(:,2);
yAxis0003=data4(:,3);
figure(11);
plotyy(yAxis0001,yAxis0003,yAxis0001,yAxis0002,'plot','plot');

%SPICE model Results - SinglePulseReset_SAMSUNG
data5=xlsread('Single_RESET_Pulse.xlsx');
yAxis0000001=data5(:,1);
yAxis0000002=data5(:,2);
yAxis0000003=data5(:,3);
yAxis0000004=data5(:,4);
yAxis0000005=data5(:,5);
yAxis0000006=data5(:,6);
yAxis0000007=data5(:,7);
figure(12);
plotyy(yAxis0000001,yAxis0000003,yAxis0000001,yAxis0000002,'plot','plot');
hold
plot(yAxis0000005,yAxis0000007);

figure(13);
plotyy(yAxis0000001,yAxis0000004,yAxis0000001,yAxis0000002,'plot','plot');
hold
plot(yAxis0000005,yAxis0000006);

```

9.1.2. MATLAB Script for $D = 3$ nm.

```

clear all, close all, clc
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Constants
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
To= 300; % Room Temperature
D = 3e-9; % Ta2O5 Thickness
Vt = 0.02585; % Thermal Voltage VT = KT/q.
Aa = 9e-10; % Electrode area
eo = 8.85418782e-12; % free space permittivity value
K=1.3806e-23;
e=1.60217646*10^(-19); % Electron Charge
KT = 0.026; % in eV
As = 120e4;
N = 1e23; % Constant
es = 27*eo; % Ta2O5 permittivity value
Phi_T = 0.0031; % (Phi_T In eV) Constant
Roff =2e4;
Ron = 1700;
Ro =12000;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Time Axis & Applied External Voltage

```

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
num_of_cycles = 1
freq = .2; %Applied bias signal frequency
tspan=[0 num_of_cycles/freq];
points=2e4; %Increase this for high indurance results
tspan_vector = linspace(tspan(1),tspan(2),points);
amp =2; % Applied bias voltage amplitude
V=zeros(size((tspan_vector)));
V = amp*sin(freq*2*pi*tspan_vector); %The applied external voltage
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%RRAM Initial Values - Initial State
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
W=zeros(size((tspan_vector)));
W_dot=zeros(size((tspan_vector)));
D_Phi=zeros(size((tspan_vector)));
Phi_s=zeros(size((tspan_vector)));
Eta=zeros(size((tspan_vector)));
Phi_B = zeros(size((tspan_vector)));
Phi_Bo = zeros(size((tspan_vector)));
Is= zeros(size((tspan_vector)));
E= zeros(size((tspan_vector)));
Vsch=zeros(size((tspan_vector)));
VD=zeros(size((tspan_vector)));
T=zeros(size((tspan_vector)));
R=zeros(size((tspan_vector)));

% The initial state of the RRAM is the fully doped state w=0 (LRS)
w_init = 0.0;
W0=w_init*D;
delta_t=tspan_vector(2)-tspan_vector(1);
W(1)=W0;

R(1) = Ron+Ro;
Itun(1) = V(1)/R(1);
T(1)=300;
Vsch(1)=(V(1)-(Itun(1).*R(1)));
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Schottky Barrier and tunneling equations
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
f=1e13;
a=1e-9;
Ea=1;
Rth=1e8;

for i=2:length(tspan_vector)

Phi_Bo(i-1)=0.45.*((W(i-1)./D));
D_Phi(i-1) = (((e^3).*N.*Phi_Bo(i-1))/((8.*(pi^2)).*es^3)).^.25);
Phi_B(i-1) = Phi_Bo(i-1) - D_Phi(i-1);

```

```

R(i-1)=(Ro+(Ron*(D-W(i-1))/D)+(Roff*W(i-1)/D));
Eta(i-1)=60000*((1000*(D-W(i-1))/D)+(900*W(i-1)/D));
    if V(i-1) < 0
        Is(i-1)=Aa*As*(To^2)*exp(-Phi_B(i-1)./(5.25*K*To/e));
        Itun(i)=Is(i-1).*(exp(Vsch(i-1)./(Eta(i-1).*Vt))-1).*exp(-W(i-
1)*1e10*sqrt(Phi_T));
    elseif V(i-1) >= 0
        Is(i-1)=Aa*As*(To^2)*exp(-Phi_B(i-1)./(2000*(K*To/e)));
        Itun(i)=-Is(i-1).*(exp(-Vsch(i-1)./(Eta(i-1).*Vt))-1).*exp(-W(i-
1)*1e10*sqrt(Phi_T));
    end;

if V(i) <= 0
Vsch(i)=(V(i)-(Itun(i).*R(i-1)));
VD(i)=(V(i)-(Itun(i).*Ro)-Vsch(i));
E(i)=VD(i)./(W(i-1)+((Ron/Roff)*(D-W(i-1))));
T(i)=To+(Rth*(Itun(i)^2*(R(i-1)-Ro)));
W_dot(i)=a*f.*exp(-Ea*e/(K*T(i))).*sinh((55*e*a*E(i))/(1*K*T(i)));
elseif V(i)>0
V(i) = 3*sin(freq*2*pi*tspan_vector(i));
Vsch(i)=(V(i)-(Itun(i).*R(i-1)));
VD(i)=(V(i)-(Itun(i).*Ro)-Vsch(i));
E(i)=VD(i)./(W(i-1)+((Ron/Roff)*(D-W(i-1))));
T(i)=To+(Rth*(Itun(i)^2*(R(i-1)-Ro)));
W_dot(i)=.6e-6*a*f.*exp(-Ea*e/(K*T(i))).*sinh((0.02*e*a*E(i))/(1*K*T(i)));
end;
W(i)=W(i-1)+W_dot(i)*delta_t;

if W(i) <= 0
    W(i) = 0;
    W_dot(i)=0;
elseif W(i) > D
    W(i) = D;
    W_dot(i)=D;
end

end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Simulation Plots
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
subplot(2,4,1)
plot(tspan_vector,W/D,'r');

subplot(2,4,2)
plot(tspan_vector,V);
title('V-t curve');
xlabel('T[Sec]');
ylabel('V[Volts]');

subplot(2,4,3)
plot(W/D,E);
title('V-E curve');
xlabel('W/D');
ylabel('E (V/m)');

```

```

subplot(2,4,4)
plot(tspan_vector,Itun);
title('I-t curve');
xlabel('T[Sec]');
ylabel('I[Amps]');

subplot(2,4,5)
plot(V,Itun);
xlabel('V1[volt]');
ylabel('It[amp]');

subplot(2,4,6)
plot(W/D,Vsch);
title('Vsch');
xlabel('T[Sec]');
ylabel('Vsch[volt]');

subplot(2,4,7)
plot(V,R);
% title('');
xlabel('Voltage(V)');
ylabel('Resistance(?)');

subplot(2,4,8)
plot(V, Phi_B);
xlabel('Voltage(V)');
ylabel('?_b[eV]');

%Matlab model Results
data=xlsread('D3nm_ExpData.xlsx');
xAxis=data(:,1);
yAxis=data(:,2);
figure(2);
semilogy(V,abs(Itun));
hold;
semilogy(xAxis,abs(yAxis));
% title('It-V1 semilogy curve');
xlabel('Voltage (V)');
ylabel('Current (V)');

%SPICE model Results
data1=xlsread('SPICE_D3nm.xlsx');
xAxis1=data1(:,1);
yAxis1=data1(:,2);
xAxis2=data1(:,3);
yAxis2=data1(:,4);
figure(3);
semilogy(xAxis1,abs(yAxis1));
hold;
semilogy(xAxis2,abs(yAxis2));
xlabel('Bias Voltage (V)');
ylabel('Current (A)');
figure(4);
semilogy(V,abs(E));
xlabel('Voltage (V)');

```

```

ylabel('E (V/m)');

%SPICE model Results-Pulse
data2=xlsread('SPICE_D3nm_Pulse.xlsx');
xAxis3=data2(:,1);
yAxis3=data2(:,2);
xAxis4=data2(:,3);
yAxis4=data2(:,4);
figure(5);
plot(xAxis3,yAxis3);
hold;
plot(xAxis4,yAxis4);
xlabel('Bias Voltage (V)');
ylabel('Current (A)');

% Linear I-V curve (Matlab Result)
figure(6);
plot(V,Itun);
xlabel('V1[volt]');
ylabel('It[amp]');

%SPICE model Results - Different Sweep Rates (SPICE Model Results)
% Make amp =3; freq = 0.2, 2, and 20 Hz
data3=xlsread('SPICE_D3nm_DifferentSweepRates.xlsx');
xAxis5=data3(:,1);
yAxis5=data3(:,2);
xAxis6=data3(:,3);
yAxis6=data3(:,4);
xAxis7=data3(:,5);
yAxis7=data3(:,6);
figure(7);
plot(xAxis5,yAxis5, 'b',xAxis6,yAxis6, 'g');
hold;
plot(xAxis7,yAxis7,'r');
xlabel('Bias Voltage (V)');
ylabel('Current (A)');

```

9.2. SPICE Subcircuit for the Proposed MISM SPICE RRAM Model Presented in Chapter Five

9.2.1. SPICE Subcircuit for $D = 4$ nm

.SUBCKT TaOxRRAM plus minus TPF Phi_b Vs PARAMS:

+T0=300 D=4e-9 VT=0.02585 Ar=9e-10 e0=8.85418782e-12

+k=1.3806e-23 q=1.60217646e-19 As=120e4 es=27*e0 N=1e23

+Phi_T=0.00175 Roff=40k Ron=1.7k Ro=12k f=1e13 a=1e-9 U=1 Rth=1e8

+x1=215 x2=0.4 v1=1 v2=0.6e-6 n1=0.1852 n2=0.0117 m=6e6

$$EV \ V \ 0 \ value = \{V(\text{plus}) - V(\text{minus})\}$$

$$E\Phi_{Bn} \ \Phi_{Bn} \ 0 \ value = \{0.6 * V(w) / D\}$$

$$ED_{\Phi} \ D_{\Phi} \ 0 \ value = \{(((q^{**3}) * N * V(\Phi_{Bn})) / (8 * (\pi^{**2}) * (es^{**3})))^{**0.25}\}$$

$$E\Phi_b \ \Phi_b \ 0 \ value = \{V(\Phi_{Bn}) - V(D_{\Phi})\}$$

$$EEta \ \eta \ 0 \ value = \{m * ((10 * (D - V(w)) / D) + (9 * V(w) / D))\}$$

$$ETPF \ TPF \ 0 \ value = \{\exp(-V(w) * \text{sqrt}(\Phi_T) * 1e10)\}$$

$$ERs \ Rs \ 0 \ value = \{Ro + (Ron * (D - V(w)) / D) + (Roff * V(w) / D)\}$$

$$EVRs \ PVs \ minus \ value = \{V(Rs) * I(EVRs)\}$$

$$EVs \ Vs \ 0 \ value = \{V(V) - (I(EVRs) * V(Rs))\}$$

*ON switching Current ($V < 0$)

$$EIsOn \ IsOn \ 0 \ value = \{stp(-V(V)) * Ar * As * (T0^{**2}) * \exp(-n1 * V(\Phi_b) / (k * T0 / q))\}$$

$$GltunON \ plus \ PVs \ value = \{V(IsOn) * (\exp(V(Vs) / (V(\eta) * VT)) - 1) * V(TPF)\}$$

$$*Eaa1 \ aa1 \ 0 \ value = \{(\exp(V(Vs) / (V(\eta) * VT)) - 1)\}$$

*OFF switching Current ($V \geq 0$)

$$EIsOff \ IsOff \ 0 \ value = \{stp(V(V)) * Ar * As * (T0^{**2}) * \exp(-n2 * V(\Phi_b) / (k * T0 / q))\}$$

$$GltunOFF \ plus \ PVs \ value = \{(-V(IsOff)) * (\exp(-V(Vs) / (V(\eta) * VT)) - 1) * V(TPF)\}$$

Dynamical Model-Differential equation modeling

$$EVD \ VD \ 0 \ value = \{V(V) - (I(EVRs) * Ro) - V(Vs)\}$$

$$EEu \ Eu \ 0 \ value = \{V(VD) / (V(w) + ((Ron / Roff) * (D - V(w))))\}$$

$$ET \ T \ 0 \ value = \{T0 + (Rth * (I(EVRs)^{**2}) * (V(Rs) - Ro))\}$$

$$EKT \ KT \ 0 \ value = \{k * V(T)\}$$

*Dynamical ON switching ($V < 0$)

Ewset wset 0 value= $\{v1 * a * f * \exp(-U * q / V(KT))\}$

Gon 0 dw/dt value= $\{V(wset) * \sinh(stp(-V(V)) * (x1 * q * a * V(Eu)) / V(KT))\}$

*Dynamical OFF switching ($V \geq 0$)

Ewreset wreset 0 value= $\{v2 * a * f * \exp(-U * q / V(KT))\}$

Goff 0 dw/dt value= $\{V(wreset) * \sinh(stp(V(V)) * (x2 * q * a * V(Eu)) / V(KT))\}$

C1 dw/dt 0 1 IC=0

R1 dw/dt 0 1e9MEG

EW w 0 value= $'((V(dw/dt) > 0) \& (V(dw/dt) < D)) ? \{V(dw/dt)\} : \{V(dw/dt) \leq 0 ? \{0\} : \{D\}\}'$

.end TaOxRRAM

9.2.2. SPICE Subcircuit for $D = 3$ nm

Model parameters

.SUBCKT TaOxRRAM plus minus PARAMS:

+To=300 D=3e-9 Vt=0.02585 Ar=9e-10 eo=8.85418782e-12

+K=1.3806e-23 e=1.60217646e-19 As=120e4 es=27*eo N=1e23

+Phi_T=0.0031 Roff=20k Ron=1.7k Ro=12k f=1e13 a=1e-9 Ea=1 Rth=1e8

+x1=95 x2=0.03

Static (nonswitching) model of the memristor

EV V 0 value= $\{V(\text{plus}) - V(\text{minus})\}$

EPhi_Bn Phi_Bn 0 value= $\{0.45 * V(w) / D\}$

ED_Phi D_Phi 0 value= $\{((e^{**3}) * N * V(\text{Phi_Bn})) / (8 * (\pi^{**2}) * (es^{**3}))^{**0.25}\}$

EPhi_b Phi_b 0 value={V(Phi_Bn)-V(D_Phi)}

EEta Eta 0 value={6e6*((10*(D-V(w))/D)+(9*V(w)/D))}

ETPF TPF 0 value={exp(-V(w)*sqrt(Phi_T)*30/D)}

ERs Rs 0 value={Ro+(Ron*(D-V(w))/D)+(Roff*V(w)/D)}

EVRs PVs minus value={V(Rs)*I(EVRs)}

EVs Vs 0 value={V(V)-(I(EVRs)*V(Rs))}

*ON switching Current (V<0)

EIsOn IsOn 0 value={stp(-V(V))*Ar*As*(To**2)*exp(-V(Phi_b)/(5.25*K*To/e))}

GltunON plus PVs value={V(IsOn)*(exp(V(Vs)/(V(Eta)*Vt))-1)*V(TPF)}

*OFF switching Current (V>=0)

EIsOff IsOff 0 value={stp(V(V))*Ar*As*(To**2)*exp(-V(Phi_b)/(85*K*To/e))}

GltunOFF plus PVs value={(-V(IsOff))*(exp(-V(Vs)/(V(Eta)*Vt))-1)*V(TPF)}

Dynamical Model-Differential equation modeling

EVD VD 0 value={V(V)-(I(EVRs)*Ro)-V(Vs)}

EERCF ERCF 0 value={V(VD)/(V(w)+((Ron/Roff)*(D-V(w))))}

ET T 0 value={To+(Rth*(I(EVRs)**2)*(V(Rs)-Ro))}

EKT KT 0 value={K*V(T)}

*Dynamical ON switching (V<0)

Ewset wset 0 value={a*f*exp(-Ea*e/V(KT))}

Gon 0 dw/dt value={V(wset)*sinh(stp(-V(V))*(95*e*a*V(ERCF))/V(KT))}

*Dynamical OFF switching (V>=0)

Ewreset wreset 0 value={0.6e-6*a*f*exp(-Ea*e/V(KT))}


```
Goff 0 dw/dt value={V(wreset)*sinh(stp(V(V))*(0.03*e*a*V(ERCF))/V(KT))}
```

```
C1 dw/dt 0 1 IC=0
```

```
R1 dw/dt 0 1e9MEG
```

```
EW w 0 value='((V(dw/dt) > 0) & (V(dw/dt) < D)) ? {V(dw/dt)} : {V(dw/dt) <= 0 ? {0} : {D}}'
```

```
.end TaOxMemristor
```